Data Provenance

David Koop Computer & Information Science University of Massachusetts Dartmouth



Scientific Publication

Galois Conjugates of Topological Phases

M. H. Freedman, ¹ J. Gukelberger, ² M. B. Hastings, ¹ S. Trebst, ¹ M. Troyer, ² and Z. Wang ¹

¹Microsoft Research, Station Q, University of California, Santa Barbara, CA 93106, USA

²Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland

(Dated: July 6, 2011)

Galois conjugation relates unitary conformal field theories (CFTs) and topological quantum field theories (TQFTs) to their non-unitary counterparts. Here we investigate Galois conjugates of quantum double models, such as the Levin-Wen model. While these Galois conjugated Hamiltonians are typically non-Hermitian, we find that their ground state wave functions still obey a generalized version of the usual code property (local operators do not act on the ground state manifold) and hence enjoy a generalized topological protection. The key question addressed in this paper is whether such non-unitary topological phases can also appear as the ground states of Hermitian Hamiltonians. Specific attempts at constructing Hermitian Hamiltonians with these ground states lead to a loss of the code property and topological protection of the degenerate ground states. Beyond this we rigorously prove that no local change of basis (IV.5) can transform the ground states of the Galois conjugated doubled Fibonacci theory into the ground states of a topological model whose Hermitian Hamiltonian satisfies Lieb-Robinson bounds. These include all gapped local or quasi-local Hamiltonians. A similar statement holds for many other non-unitary TQFTs. One consequence is that the "Gaffnian" wave function cannot be the ground state of a gapped fractional quantum Hall state.

PACS numbers: 05.30.Pr, 73.43.-f

Galois conjugation, by definition, replaces a root of a polynomial by another one with identical algebraic properties. For example, i and -i are Galois conjugate (consider $z^2+1=0$) as are $\phi=\frac{1+\sqrt{5}}{2}$ and $-\frac{1}{\phi}=\frac{1-\sqrt{5}}{2}$ (consider $z^2-z-1=0$), as well as $\sqrt[3]{2}$, $\sqrt[3]{2}e^{2\pi i/3}$, and $\sqrt[3]{2}e^{-2\pi i/3}$ (consider $z^3-2=0$). In physics Galois conjugation can be used to convert nonunitary conformal field theories (CFTs) to unitary ones, and vice versa. One famous example is the non-unitary Yang-Lee CFT, which is Galois conjugate to the Fibonacci CFT $(G_2)_1$, the even (or integer-spin) subset of su(2) $_3$.

I. INTRODUCTION

In statistical mechanics non-unitary conformal field theories have a venerable history. 1,2 However, it has remained less clear if there exist physical situations in which non-unitary models can provide a useful description of the low energy physics of a quantum mechanical system - after all, Galois conjugation typically destroys the Hermitian property of the Hamiltonian. Some non-Hermitian Hamiltonians, which surprisingly have totally real spectrum, have been found to arise in the study of PT-invariant one-particle systems³ and in some Galois conjugate many-body systems⁴ and might be seen to open the door a crack to the physical use of such models. Another situation, which has recently attracted some interest, is the question whether non-unitary models can describe 1D edge states of certain 2D bulk states (the edge holographic for the bulk). In particular, there is currently a discussion on whether or not the "Gaffnian" wave function could be the ground state for a gapped fractional quantum Hall (FQH) state albeit with a non-unitary "Yang-Lee" CFT describing its edge. 5-7 We conclude that this is not possible, further restricting the possible scope of non-unitary models in quantum me-

We reach this conclusion quite indirectly. Our main thrust is the investigation of Galois conjugation in the simplest nonAbelian Levin-Wen model. This model, which is also called "DFib", is a topological quantum field theory (TQFT) whose states are string-nets on a surface labeled by either a trivial or "Fibonacci" anyon. From this starting point, we give a rigorous argument that the "Gaffnian" ground state cannot be locally conjugated to the ground state of any topological phase, within a Hermitian model satisfying Lieb-Robinson (LR) bounds (which includes but is not limited to gapped local and quasi-local Hamiltonians).

Lieb-Robinson bounds are a technical tool for local lattice models. In relativistically invariant field theories, the speed of light is a strict upper bound to the velocity of propagation. In lattice theories, the LR bounds provide a similar upper bound by a velocity called the LR velocity, but in contrast to the relativistic case there can be some exponentially small "leakage" outside the light-cone in the lattice case. The Lieb-Robinson bounds are a way of bounding the leakage outside the light-cone. The LR velocity is set by microscopic details of the Hamiltonian, such as the interaction strength and range. Combining the LR bounds with the spectral gap enables us to prove locality of various correlation and response functions. We will call a Hamiltonian a *Lieb-Robinson Hamiltonian* if it satisfies

We work primarily with a single example, but it should be clear that the concept of Galois conjugation can be widely applied to TQFTs. The essential idea is to retain the particle types and fusion rules of a unitary theory but when one comes to writing down the algebraic form of the F-matrices (also called 6j symbols), the entries are now Galois conjugated. A slight complication, which is actually an asset, is that writing an F-matrix requires a gauge choice and the most convenient choice may differ before and after Galois conjugation.

Our method is not restricted to Galois conjugated DFib^{\mathcal{G}} and its factors Fib^{\mathcal{G}} and Fib^{\mathcal{G}}, but can be generalized to infinitely many non-unitary TQFTs, showing that they will not arise as low energy models for a gapped 2D quantum mechan-

non-Hermitian DYL model

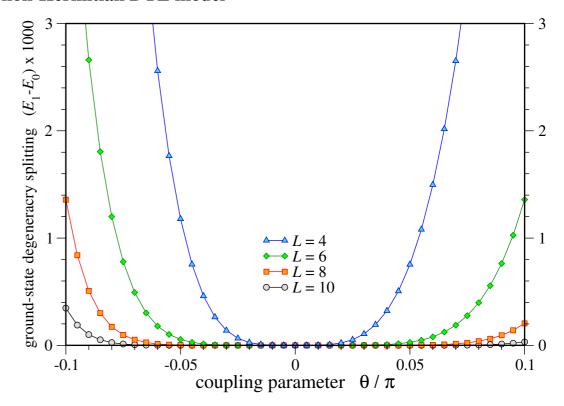
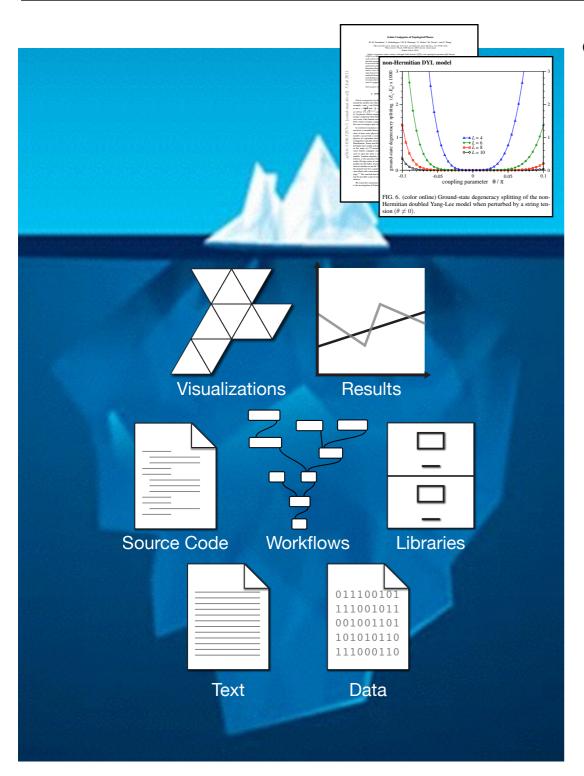


FIG. 6. (color online) Ground-state degeneracy splitting of the non-Hermitian doubled Yang-Lee model when perturbed by a string tension ($\theta \neq 0$).

["Galois Conjugates of Topological Phases", Freedman et al., 2012]

Scientific Publication

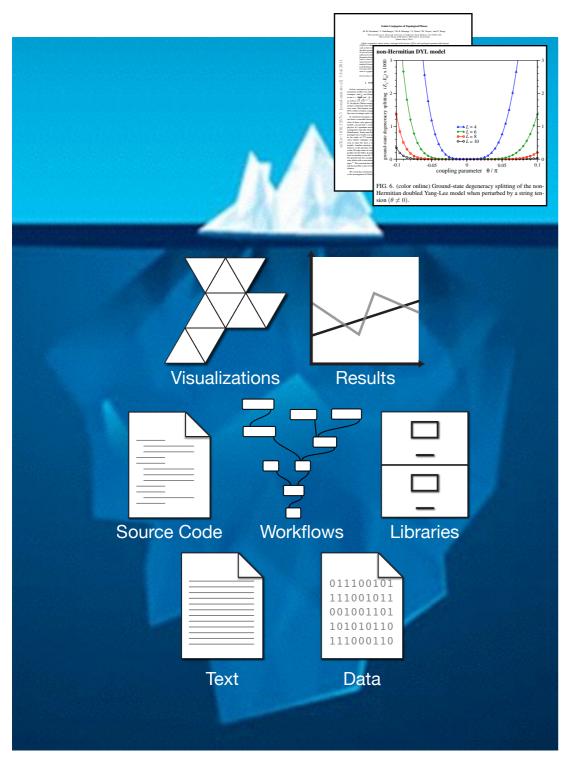


- Think about regenerating a figure from a paper written two years ago
 - Do you have the input data?
 - Do you know what software you used? Do you need to install it?
 - Does the software run on your current machine? Did the interfaces change?
 - Can you recreate the workflow/script?
 - How do you set the parameters?
 - Does everything run but you get a different result?
 - Is there a parameter/data file you forgot to record?

Reproducibility



Reproducibility



- Capture how results were achieved
- Includes many different items
- Improve community collaboration and sharing



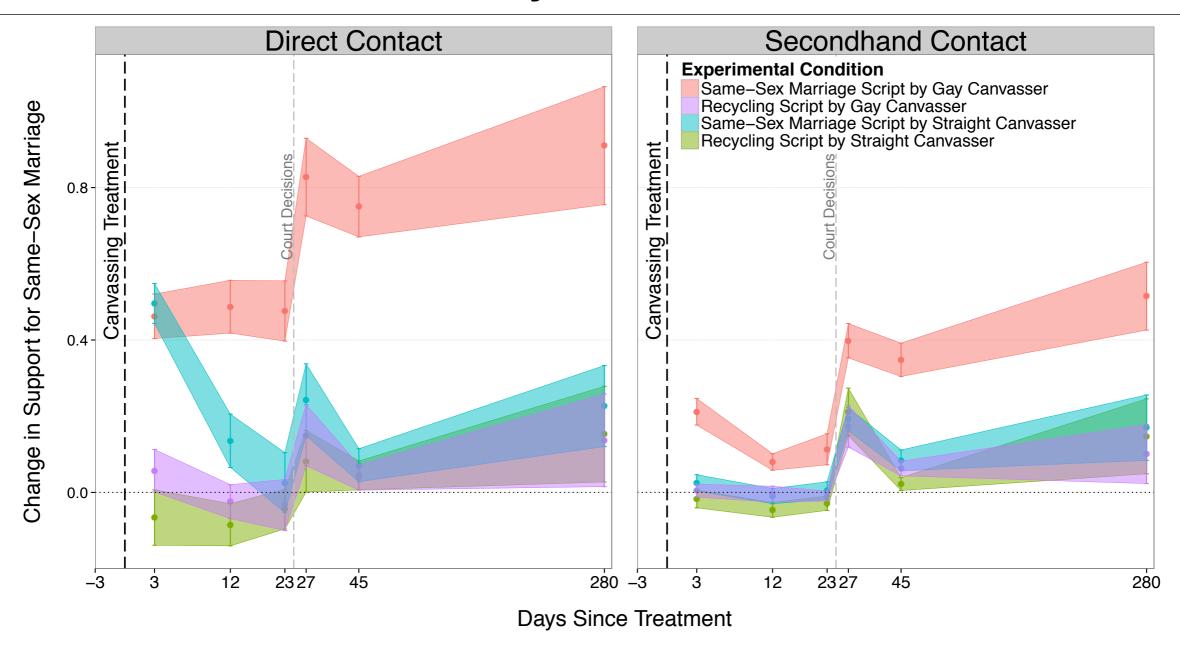


Ensure Quality, Reliability, & Trustworthiness



[Pentium Chip with FDIV Bug, Photo by Konstantin Lanzet, CC BY-SA 3.0]

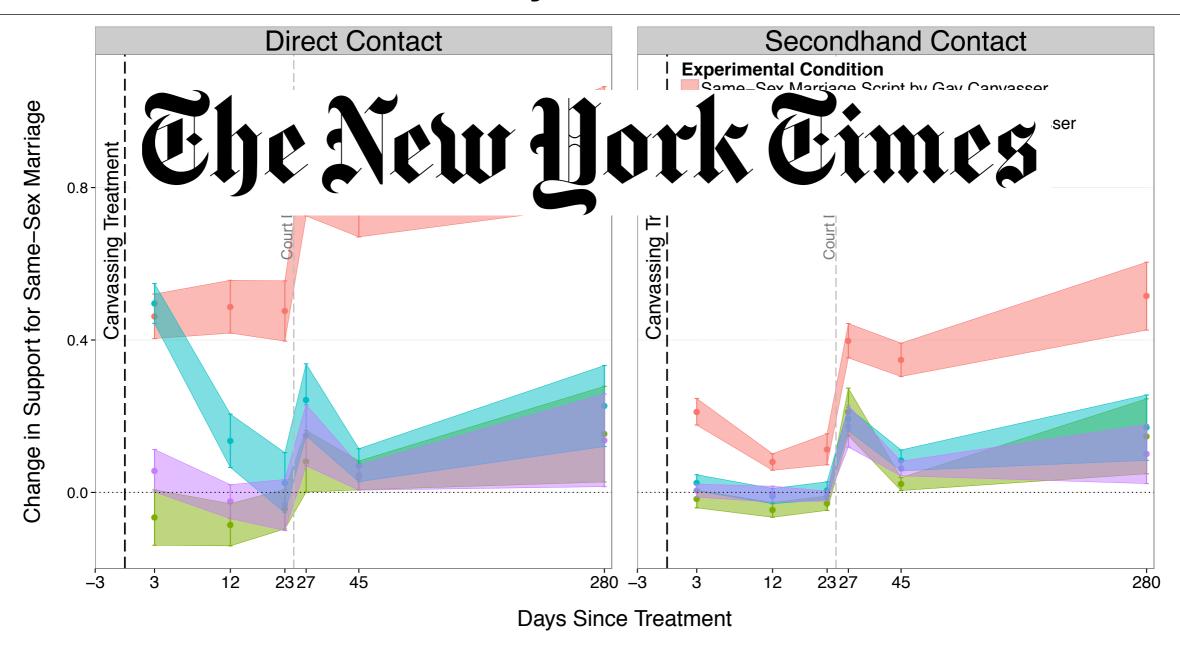
Political Science Study in the News



Note: The first vertical dashed line represents the canvassing intervention, which was administered between Internet survey waves 1 and 2. The second vertical dashed line represents the U.S. Supreme Court decisions striking down California's ban on same-sex marriage. The Y-axis is opinion change between the baseline survey and subsequent survey waves, with higher scores indicating more support for same-sex marriage. Points represent mean values, bars display 95% bootstrap confidence intervals.

[LaCour and Green, Science, 2014 (Retracted 2015)]

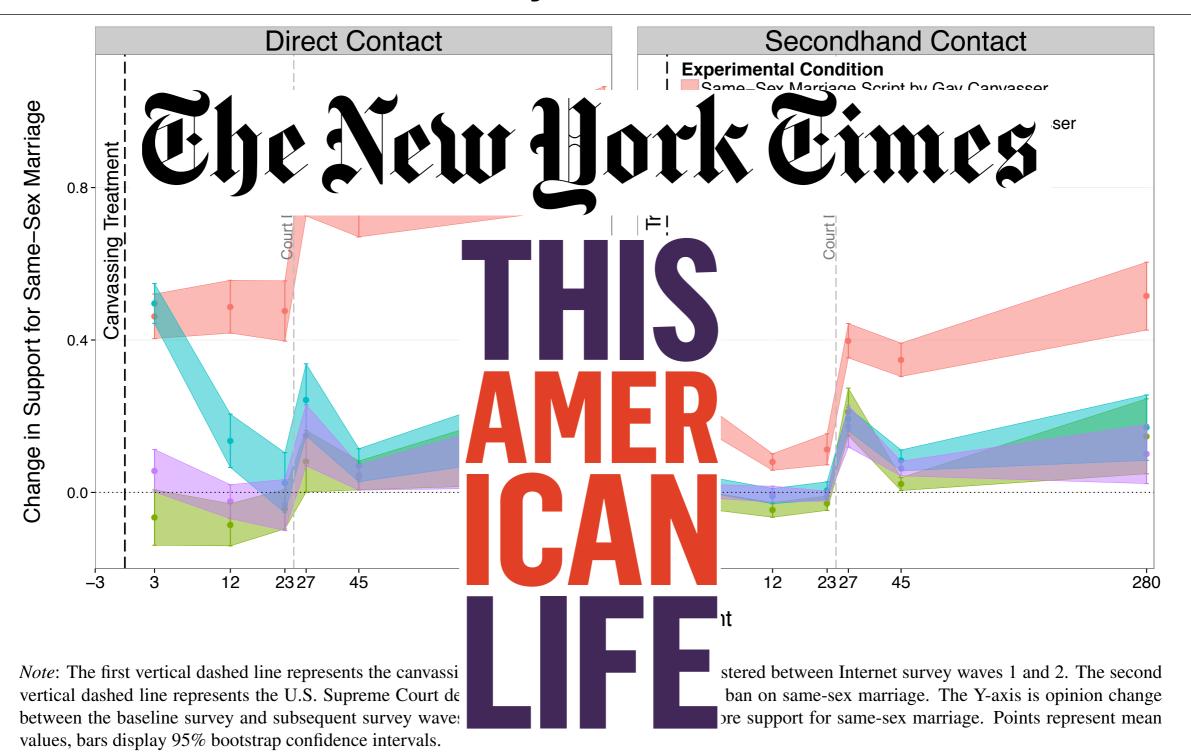
Political Science Study in the News



Note: The first vertical dashed line represents the canvassing intervention, which was administered between Internet survey waves 1 and 2. The second vertical dashed line represents the U.S. Supreme Court decisions striking down California's ban on same-sex marriage. The Y-axis is opinion change between the baseline survey and subsequent survey waves, with higher scores indicating more support for same-sex marriage. Points represent mean values, bars display 95% bootstrap confidence intervals.

[LaCour and Green, Science, 2014 (Retracted 2015)]

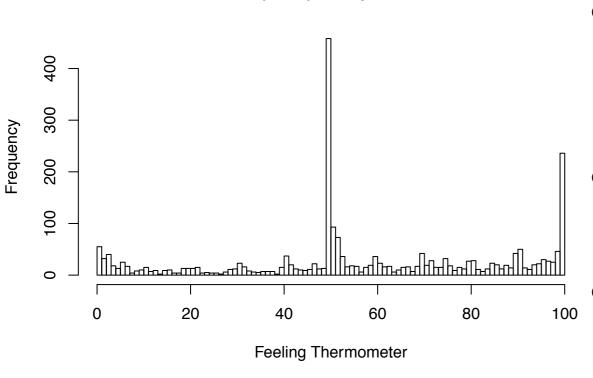
Political Science Study in the News



[LaCour and Green, Science, 2014 (Retracted 2015)]

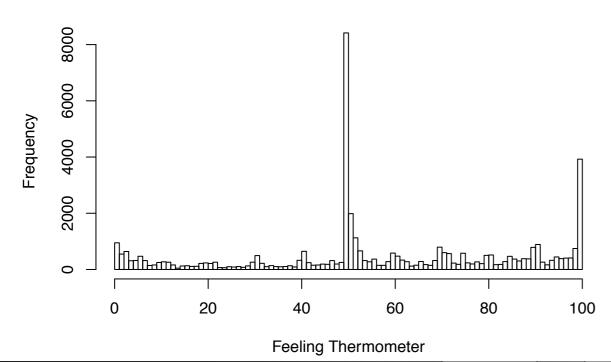
Reproducing Results

LaCour (2014) Study 2, Baseline



CCAP

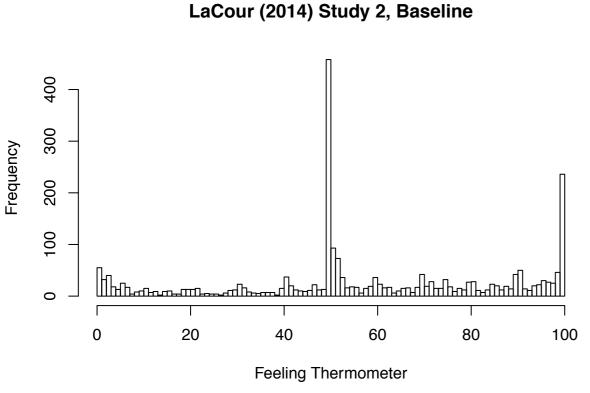
- "Irregularities in LaCour (2014)",
 Broockman, Kalla, and Aronow,
 2015
- Tried their own pilot study and were unable to get similar results
- Found published data matched other data from different studies



[Broockman et al., 2015]



Reproducing Results



- "Irregularities in LaCour (2014)", Broockman, Kalla, and Aronow, 2015
- Tried their own pilot study and were unable to get similar results
- Found published data matched other data from different studies

Remaining Uncertainties

- We do not have access to the same-sex marriage question in CCAP, so we cannot evaluate the similarities of LaCour (2014)'s same-sex marriage question to the CCAP on that item.
- The claimed treatment effect was heterogeneous by canvasser attributes and the posted replication file does not have canvasser identifiers, so it is difficult to perform diagnostics on the responses of those assigned to treatment.
- The data for the abortion study reported at http://www.cis.ethz.ch/content/dam/ethz/special-interest/ gess/cis/cis-dam/CIS_DAM_2015/Colloquium/Papers/LaCour_2015.pdf in LaCour (2015) is not currently publicly available.

Feeling Thermometer

[Broockman et al., 2015]

100

Retraction

Memo

May 19, 2015

To: Gilbert Chin From: Donald Green

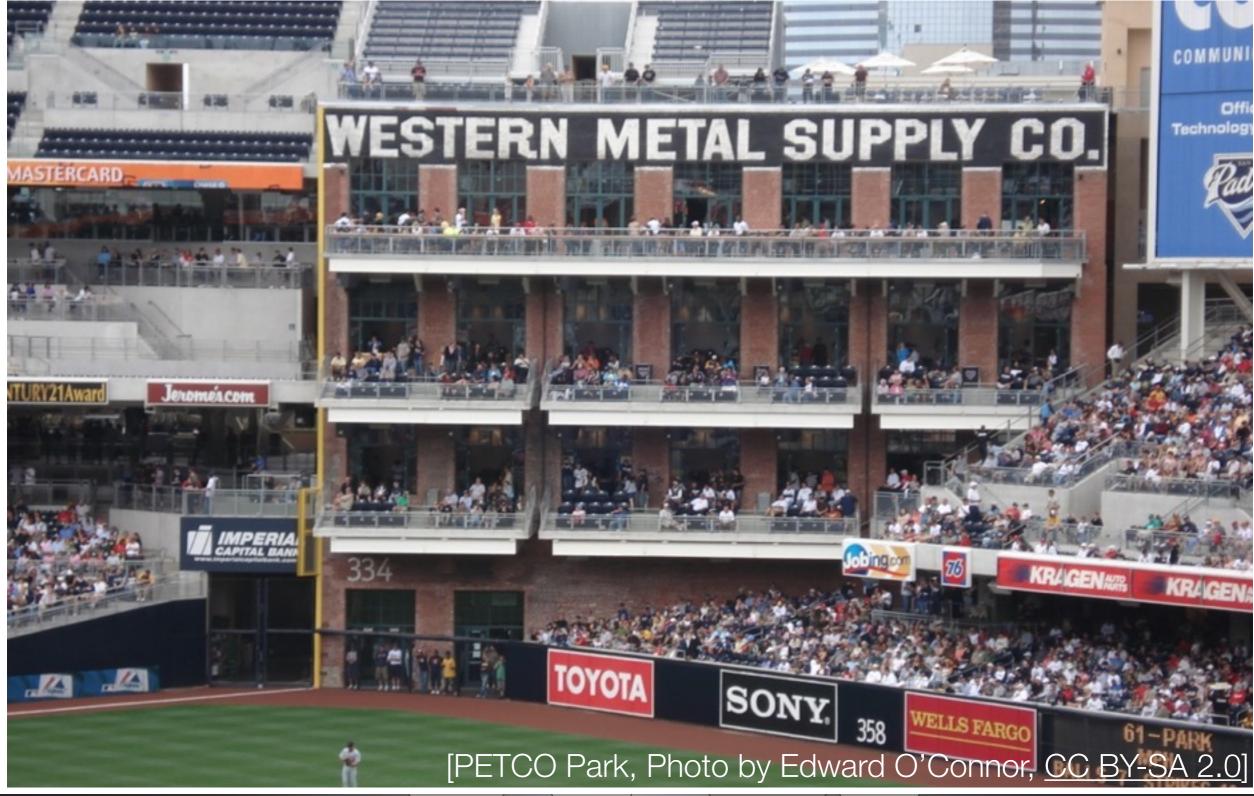
Re: Retraction of "LaCour, Michael J., and Donald P. Green. 2014. When Contact Changes Minds: An Experiment on Transmission of Support for Gay Equality. *Science*. 346(6215): 1366-1369."

I write to request a retraction of the above Science report. Last weekend, two UC Berkeley graduate students (David Broockman, and Josh Kalla) who had been working on a research project patterned after the studies reported in our article brought to my attention a series of irregularities that called into question the integrity of the data we present. They crafted a technical report with the assistance of Yale professor, Peter Aronow, and presented it to me last weekend. The report is attached. I brought their report to the attention of Lynn Vavreck, Professor of Political Science at UCLA and Michael LaCour's graduate advisor, who confronted him with these allegations on Monday morning, whereupon it was discovered that the on-line survey data that Michael LaCour purported to collect could not be traced to any originating Qualtrics source files. He claimed that he deleted the source file accidentally, but a Qualtrics service representative who examined the account and spoke with UCLA Political Science Department Chair Jeffrey Lewis reported to him that she found no evidence of such a deletion. On Tuesday, Professor Vavreck asked Michael LaCour for the contact information of survey respondents so that their participation in the survey could be verified, but he declined to furnish this information. With respect to the implementation of the surveys, Professor Vavreck was informed that, contrary to the description in the Supplemental Information, no cash incentives were offered or paid to respondents, and that, notwithstanding Michael LaCour's funding acknowledgement in the published report, he told Professor Vavreck that he did not in fact accept or use grant money to conduct surveys for either study, which she independently confirmed with the UCLA Law School and the UCLA Grants Office. Michael LaCour's failure to produce the raw data coupled with the other concerns noted above undermines the credibility of the findings.

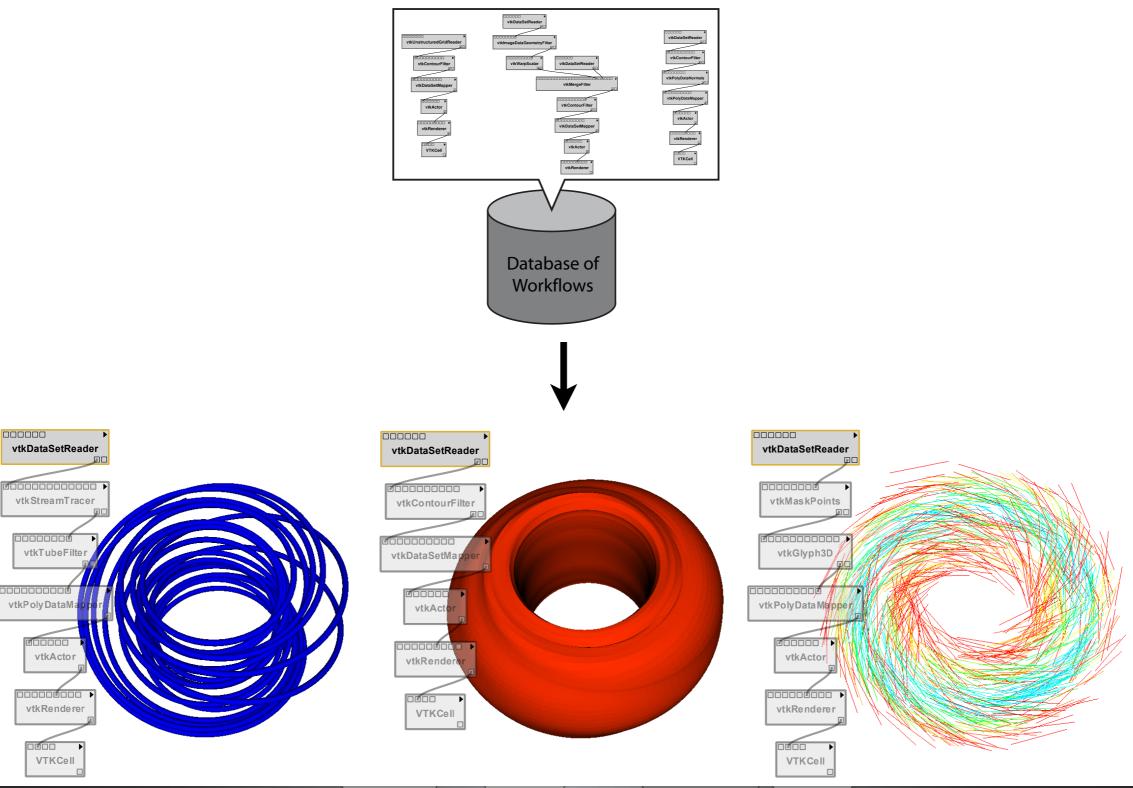
I am deeply embarrassed by this turn of events and apologize to the editors, reviewers, and readers of Science.

- Green, one of the two authors, requested retraction after these questions arose
- "...survey data could not be traced to any originating Qualtrics source files" (emphasis added)
- "...failure to produce the raw data coupled with the other concerns noted above undermines the credibility of the findings" (emphasis added)
- Science retracted the paper on May 28, 2015

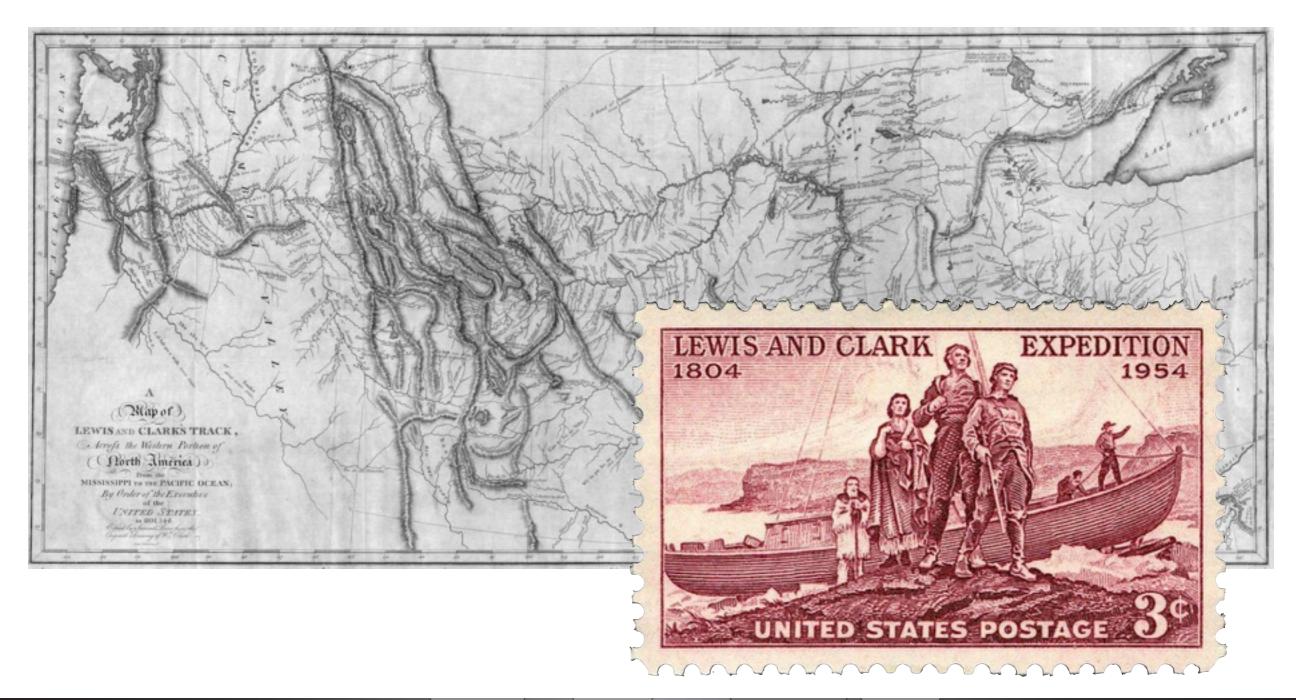
Reuse Past Work



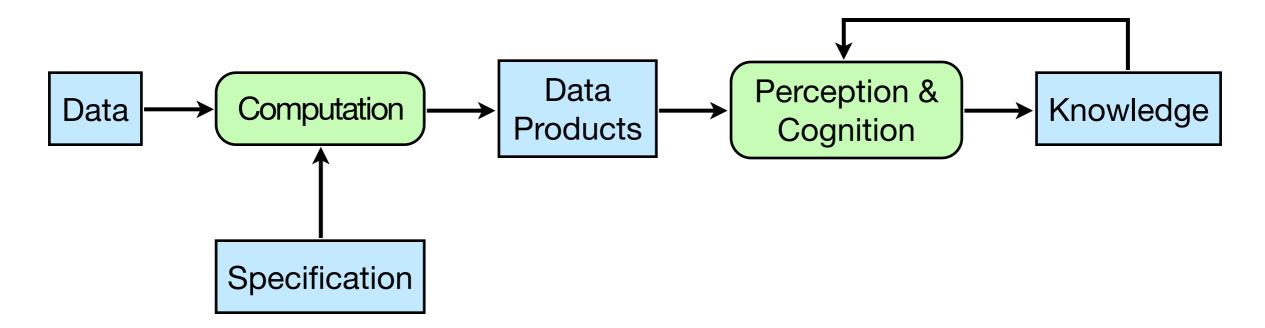
Reuse Past Work



Unencumbered Exploration & Learning

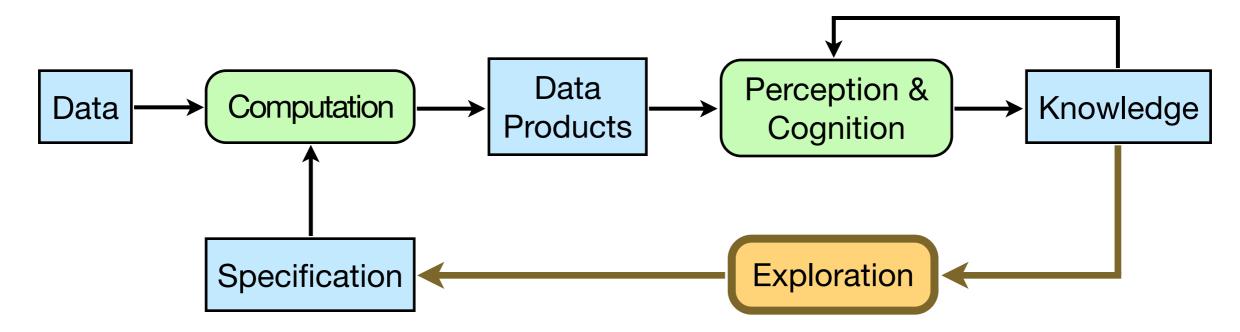


Data Exploration



[Modified from Van Wijk, Vis 2005]

Data Exploration



[Modified from Van Wijk, Vis 2005]

- Data analysis and visualization are iterative processes
- In exploratory tasks, change is the norm!

Exploration and Creativity Support

- Reasoning is key to the exploratory processes
- "Reflective reasoning requires the ability to store temporary results, to make inferences from stored knowledge, and to follow chains of reasoning backward and forward, sometimes backtracking when a promising line of thought proves to be unfruitful. ...the process is slow and laborious" — Donald A. Norman
- Need external aids—tools to facilitate this process
 - Creativity support tools [Ben Shneiderman]
- Need aid from people—collaboration

Provenance in Art



Rembrandt van Rijn
Dutch, 1606 - 1669
Self-Portrait, 1659
oil on canvas
Andrew W. Mellon Collection
1937.1.72

Provenance

George, 3rd Duke of Montagu and 4th Earl of Cardigan [d. 1790], by 1767;[1] by inheritance to his daughter, Lady Elizabeth, wife of Henry, 3rd Duke of Buccleuch of Montagu House, London; John Charles, 7th Duke of Buccleuch; (P. & D. Colnaghi & Co., New York, 1928); (M. Knoedler & Co., New York); sold January 1929 to Andrew W. Mellon, Pittsburgh and Washington, D.C.; deeded 28 December 1934 to The A.W. Mellon Educational and Charitable Trust, Pittsburgh; gift 1937 to NGA.

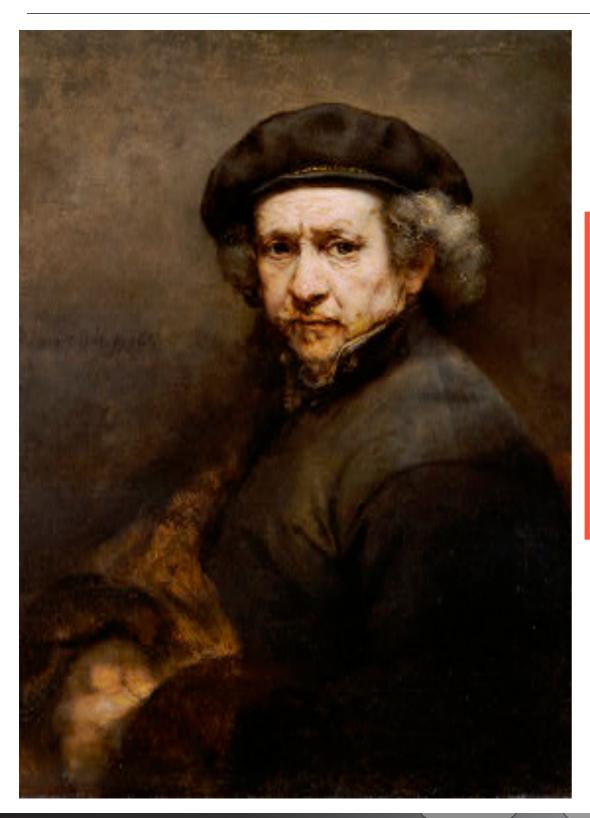
[1] This early provenance is established by presence of a mezzotint after the portrait by R. Earlom (1743-1822), dated 1767. See John Charrington, A Catalogue of the Mezzotints After, or Said to Be After, Rembrandt, Cambridge, 1923, no. 49.

Associated Names

- · Buccleuch, Henry, 3rd Duke of
- · Buccleuch, John Charles, 7th Duke of
- Colnaghi & Co., Ltd., P. & D.
- Knoedler & Company, M.
- Mellon, Andrew W.
- Mellon Educational and Charitable Trust, The A.W.
- Montagu, and 4th Earl of Cardigan, George, 3rd Duke of

[National Gallery of Art]

Provenance in Art



Rembrandt van Rijn
Dutch, 1606 - 1669
Self-Portrait, 1659
oil on canvas
Andrew W. Mellon Collection
1937.1.72

Provenance

George, 3rd Duke of Montagu and 4th Earl of Cardigan [d. 1790], by 1767;[1] by inheritance to his daughter, Lady Elizabeth, wife of Henry, 3rd Duke of Buccleuch of Montagu House, London; John Charles, 7th Duke of Buccleuch; (P. & D. Colnaghi & Co., New York, 1928); (M. Knoedler & Co., New York); sold January 1929 to Andrew W. Mellon, Pittsburgh and Washington, D.C.; deeded 28 December 1934 to The A.W. Mellon Educational and Charitable Trust, Pittsburgh; gift 1937 to NGA.

[1] This early provenance is established by presence of a mezzotint after the portrait by R. Earlom (1743-1822), dated 1767. See John Charrington, A Catalogue of the Mezzotints After, or Said to Be After, Rembrandt, Cambridge, 1923, no. 49.

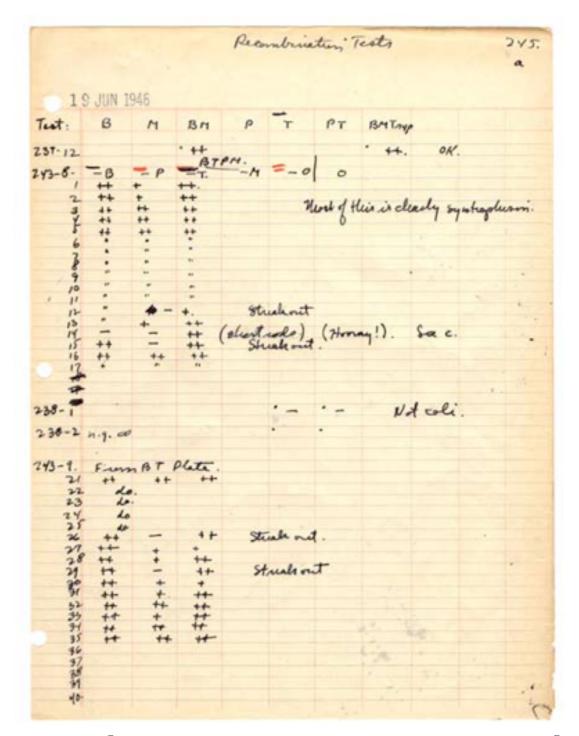
Associated Names

- · Buccleuch, Henry, 3rd Duke of
- · Buccleuch, John Charles, 7th Duke of
- Colnaghi & Co., Ltd., P. & D.
- Knoedler & Company, M.
- Mellon, Andrew W.
- Mellon Educational and Charitable Trust, The A.W.
- Montagu, and 4th Earl of Cardigan, George, 3rd Duke of

[National Gallery of Art]

Provenance in Science

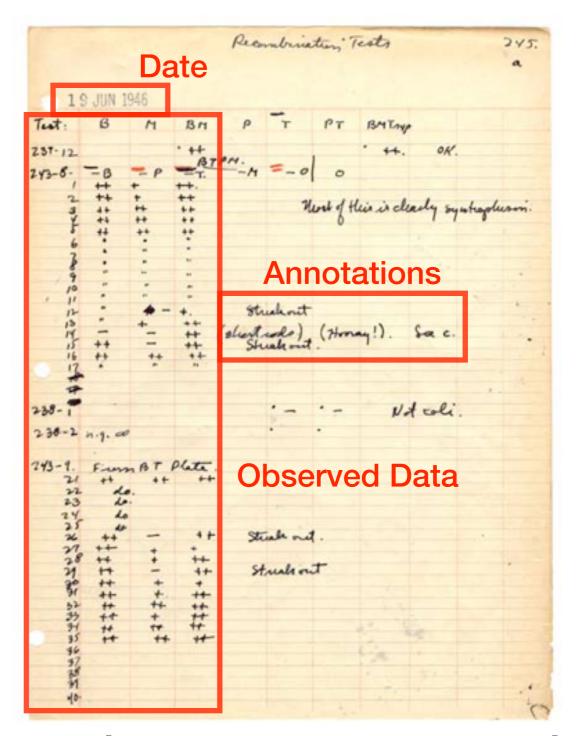
- Provenance: the lineage of data, a computation, or a visualization
- Provenance is as (or more) important as the result!
- Old solution:
 - Lab notebooks
- New problems:
 - Large volumes of data
 - Complex analyses
 - Writing notes doesn't scale



[DNA Recombination, Lederberg]

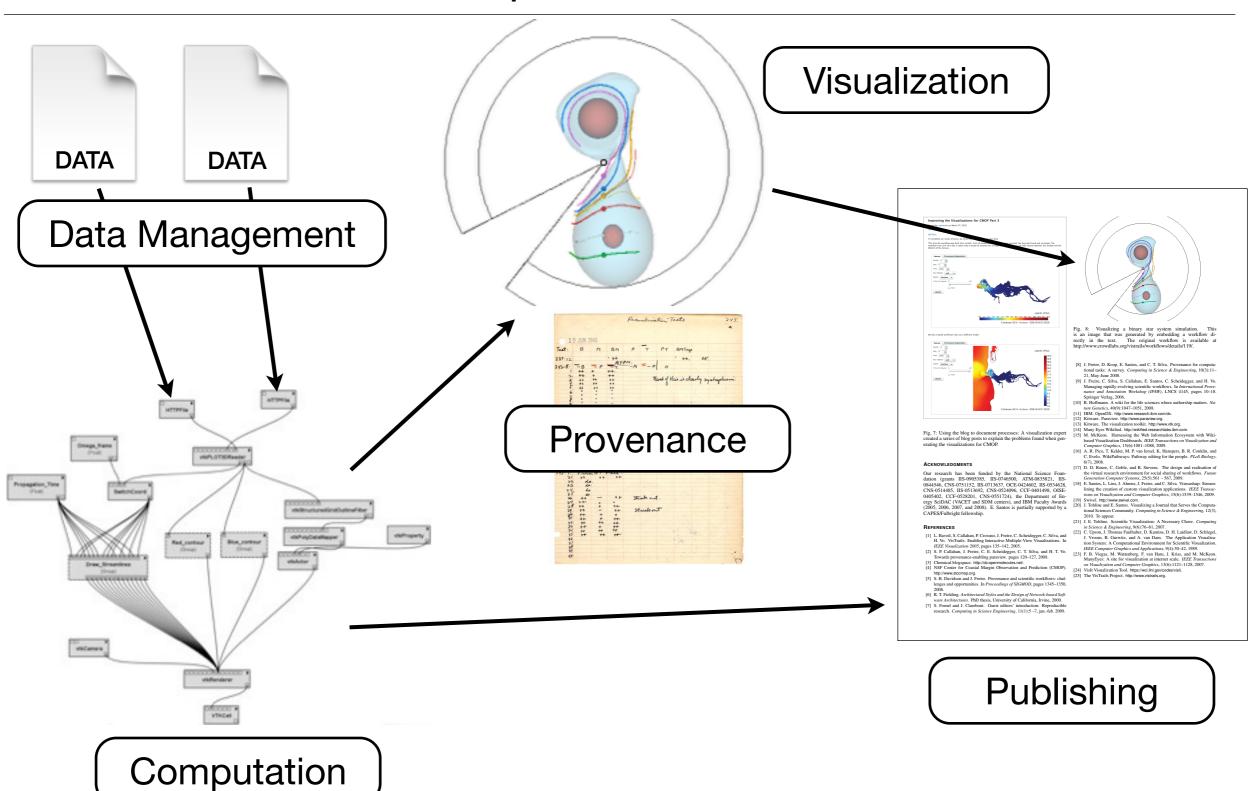
Provenance in Science

- Provenance: the lineage of data, a computation, or a visualization
- Provenance is as (or more) important as the result!
- Old solution:
 - Lab notebooks
- New problems:
 - Large volumes of data
 - Complex analyses
 - Writing notes doesn't scale



[DNA Recombination, Lederberg]

Provenance in Computational Science



Evolution of Publication

- Publish paper
- Publish code
- Publish computational experiments/tests
- Publish provenance (what actually happens during your runs)

Provenance-Rich Publication

Galois Conjugates of Topological Phases

M. H. Freedman, J. Gukelberger, M. B. Hastings, S. Trebst, M. Troyer, and Z. Wang Microsoft Research, Station Q, University of California, Santa Barbara, CA 93106, USA Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland (Dated: July 6, 2011)

Galois conjugation relates unitary conformal field theories (CFTs) and topological quantum field theories (TQFTs) to their non-unitary counterparts. Here we investigate Galois conjugates of quantum double models, such as the Levin-Wen model. While these Galois conjugated Hamiltonians are typically non-Hermitian, we find that their ground state wave functions still obey a generalized version of the usual code property (local operators do not act on the ground state manifold) and hence enjoy a generalized topological protection. The key question addressed in this paper is whether such non-unitary topological phases can also appear as the ground states of Hermitian Hamiltonians. Specific attempts at constructing Hermitian Hamiltonians with these ground states lead to a loss of the code property and topological protection of the degenerate ground states. Beyond this we rigorously prove that no local change of basis (IV.5) can transform the ground states of the Galois conjugated doubled Fibonacci theory into the ground states of a topological model whose Hermitian Hamiltonian satisfies Lieb-Robinson bounds. These include all gapped local or quasi-local Hamiltonians. A similar statement holds for many other non-unitary TQFTs. One consequence is that the "Gaffnian" wave function cannot be the ground state of a gapped fractional quantum Hall state.

PACS numbers: 05.30.Pr, 73.43.-f

I. INTRODUCTION

Galois conjugation, by definition, replaces a root of a polynomial by another one with identical algebraic properties. For example, i and -i are Galois conjugate (consider $z^2+1=0$) as are $\phi=\frac{1+\sqrt{5}}{2}$ and $-\frac{1}{\phi}=\frac{1-\sqrt{5}}{2}$ (consider $z^2-z-1=0$), as well as $\sqrt[3]{2}$, $\sqrt[3]{2}e^{2\pi i/3}$, and $\sqrt[3]{2}e^{-2\pi i/3}$ (consider $z^3-2=0$). In physics Galois conjugation can be used to convert nonunitary conformal field theories (CFTs) to unitary ones, and vice versa. One famous example is the non-unitary Yang-Lee CFT, which is Galois conjugate to the Fibonacci CFT $(G_2)_1$, the even (or integer-spin) subset of su(2) $_3$.

In statistical mechanics non-unitary conformal field theories have a venerable history. 1,2 However, it has remained less clear if there exist physical situations in which non-unitary models can provide a useful description of the low energy physics of a quantum mechanical system - after all, Galois conjugation typically destroys the Hermitian property of the Hamiltonian. Some non-Hermitian Hamiltonians, which surprisingly have totally real spectrum, have been found to arise in the study of PT-invariant one-particle systems³ and in some Galois conjugate many-body systems⁴ and might be seen to open the door a crack to the physical use of such models. Another situation, which has recently attracted some interest, is the question whether non-unitary models can describe 1D edge states of certain 2D bulk states (the edge holographic for the bulk). In particular, there is currently a discussion on whether or not the "Gaffnian" wave function could be the ground state for a *gapped* fractional quantum Hall (FQH) state albeit with a non-unitary "Yang-Lee" CFT describing its edge.⁵⁻⁷ We conclude that this is not possible, further restricting the possible scope of non-unitary models in quantum me-

We reach this conclusion quite indirectly. Our main thrust is the investigation of Galois conjugation in the simplest non-

Abelian Levin-Wen model. This model, which is also called "DFib", is a topological quantum field theory (TQFT) whose states are string-nets on a surface labeled by either a trivial or "Fibonacci" anyon. From this starting point, we give a rigorous argument that the "Gaffnian" ground state cannot be locally conjugated to the ground state of any topological phase, within a Hermitian model satisfying Lieb-Robinson (LR) bounds (which includes but is not limited to gapped local and quasi-local Hamiltonians).

Lieb-Robinson bounds are a technical tool for local lattice models. In relativistically invariant field theories, the speed of light is a strict upper bound to the velocity of propagation. In lattice theories, the LR bounds provide a similar upper bound by a velocity called the LR velocity, but in contrast to the relativistic case there can be some exponentially small "leakage" outside the light-cone in the lattice case. The Lieb-Robinson bounds are a way of bounding the leakage outside the light-cone. The LR velocity is set by microscopic details of the Hamiltonian, such as the interaction strength and range. Combining the LR bounds with the spectral gap enables us to prove locality of various correlation and response functions. We will call a Hamiltonian a *Lieb-Robinson Hamiltonian* if it satisfies

We work primarily with a single example, but it should be clear that the concept of Galois conjugation can be widely applied to TQFTs. The essential idea is to retain the particle types and fusion rules of a unitary theory but when one comes to writing down the algebraic form of the F-matrices (also called 6j symbols), the entries are now Galois conjugated. A slight complication, which is actually an asset, is that writing an F-matrix requires a gauge choice and the most convenient choice may differ before and after Galois conjugation.

Our method is not restricted to Galois conjugated DFib^{\mathcal{G}} and its factors Fib^{\mathcal{G}} and $\overline{\text{Fib}}^{\mathcal{G}}$, but can be generalized to infinitely many non-unitary TQFTs, showing that they will not arise as low energy models for a gapped 2D quantum mechan-

non-Hermitian DYL model

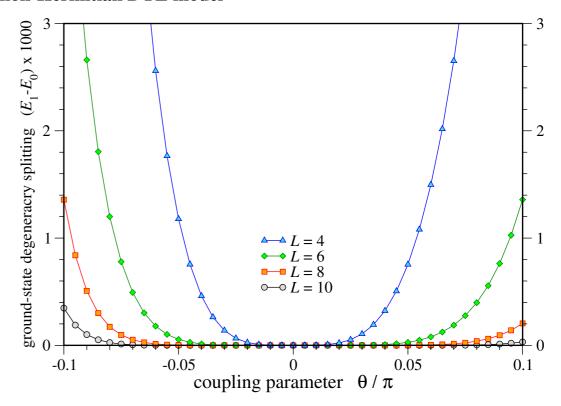


FIG. 6. (color online) Ground-state degeneracy splitting of the non-Hermitian doubled Yang-Lee model when perturbed by a string tension ($\theta \neq 0$).

[Freedman et al., 2012]

Benefits of Provenance-Rich Publications

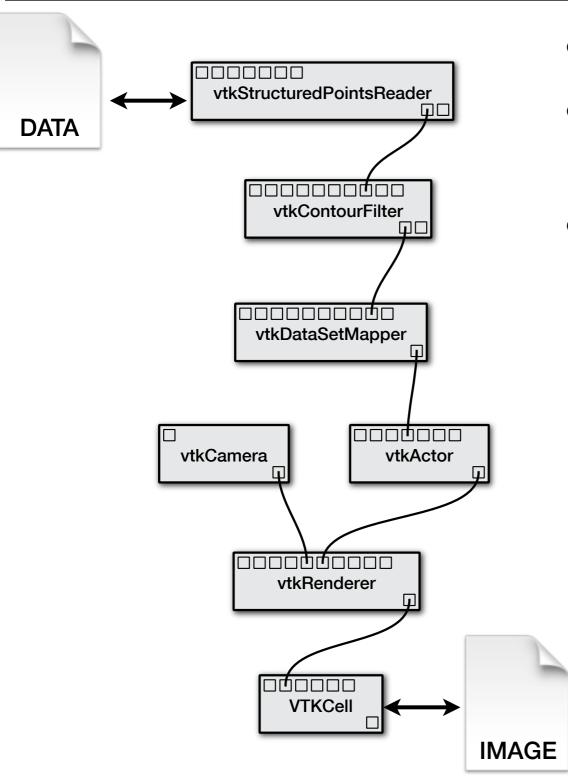
- Produce more knowledge-not just text
- Allow scientists to stand on the shoulders of giants (and their own)
- Science can move faster!
- Higher-quality publications
- Authors will be more careful
- Many eyes to check results
- Describe more of the discovery process: people only describe successes, can we learn from mistakes?
- Expose users to different techniques and tools: expedite their training; and potentially reduce their time to insight

ATPESC 2015

Provenance Definitions

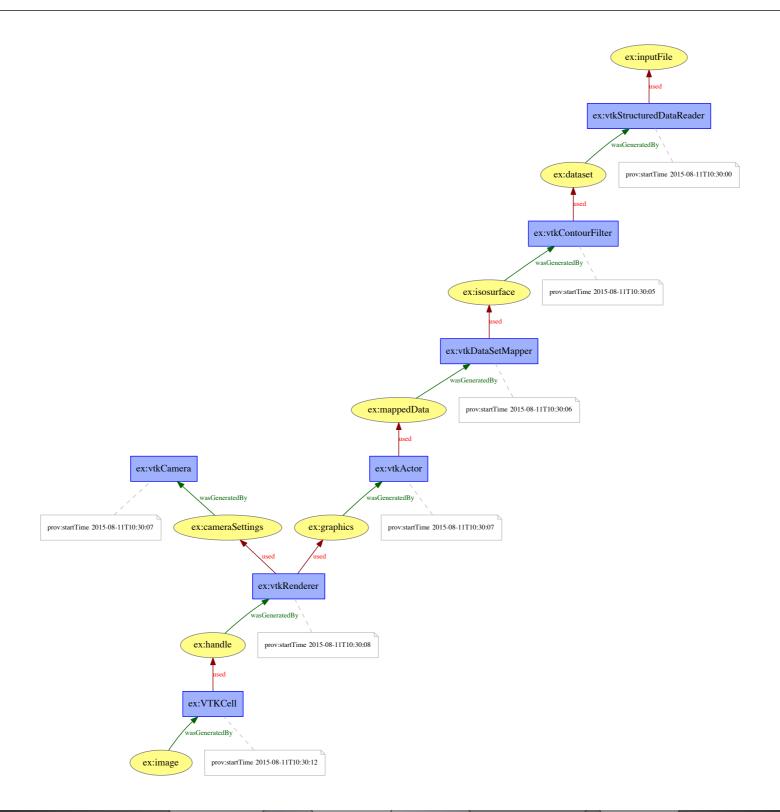
- Dictionary: "the source or origin of an object; its history and pedigree; a record of the ultimate derivation and passage of an item through its various owners."
- Focus on causality—the sequence of steps that detail how a result was generated and/or derivation—what data a result depended on
- Provenance itself is data, this list of steps along with metadata for each step: when it occurred, who initiated it, notes about it
- Can be used to preserve information about an experiment and to answer many questions

Workflows

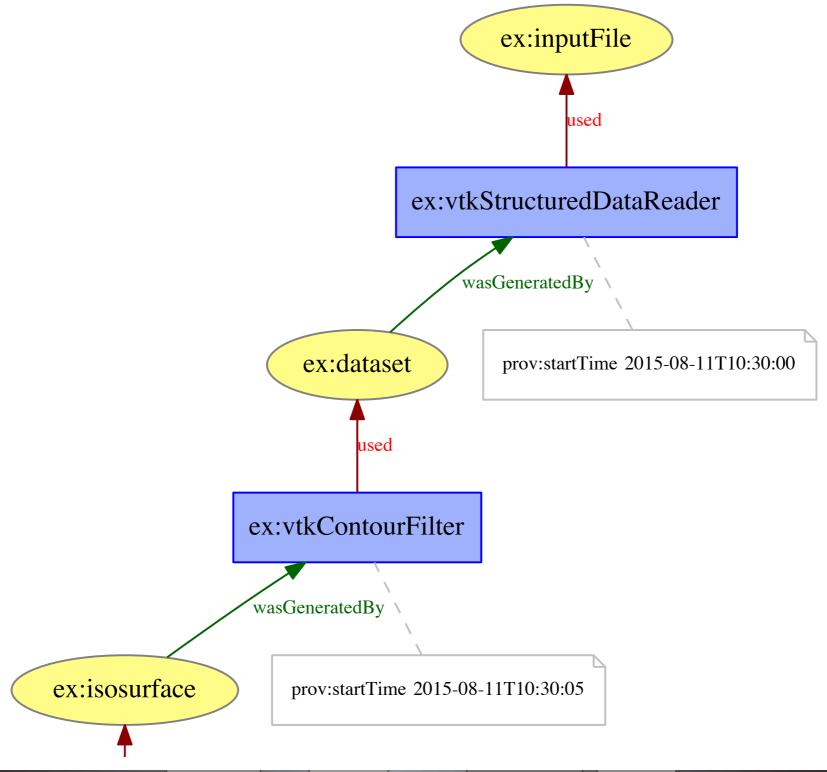


- Abstract computation
- Computational modules connected through input and output ports
- Data flows along the connections

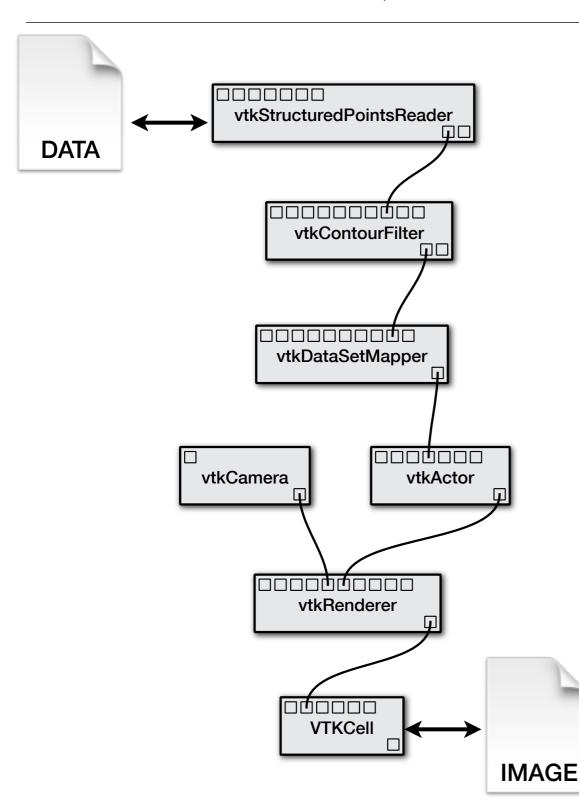
Provenance Graph



Provenance Graph



Provenance Questions



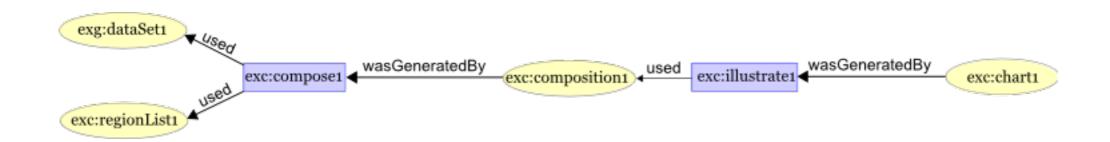
- What process led to the output image?
- What input datasets contributed to the output image?
- What workflows create an isosurface with isovalue 57?
- Who create this data product?
- When was this data file created?
- Why was vtkCamera used?
- Why do two output images differ?

Provenance Management

- Provenance can be generated from tasks/programs/scripts/etc.
- Properties of provenance is related to the computational model
 - a specific application with a graphical interface
 - a script that automates the use of several command-line tools
 - a scientific workflow that combines several tools

Provenance & Causality

- Knowing what data/steps influenced other data/steps is important!
- Data dependencies: this output file depended on this input file
- Data-process dependencies: this output figure depended on these processes
- Causality can often be represented as a graph where connections represent dependencies



User-defined provenance

- Goal: capture lots of provenance automatically based on what steps are executed
- Problem: not everything can be captured automatically
- Annotations offer ability to keep notes about processes
- Users might also specify known causal links that cannot be automatically determined (e.g. a step depends on three system files that were not specified as inputs in the workflow)

Provenance Management

- What is needed to capture, store, and use provenance?
 - 1. Capture mechanism
 - 2. Model for representing provenance
 - 3. Tools to store, query, and analyze provenance

Provenance Capture Mechanisms

Workflow-based

- Since workflow execution is controlled, keep track of all the workflow modules, parameters, etc. as they are executed

Process-based

- Each process is required to write out its own provenance information (not centralized like workflow-based)

OS-based

- The OS or filesystem is modified so that any activity it does it monitored and the provenance subsystem organizes it

• Tradeoffs:

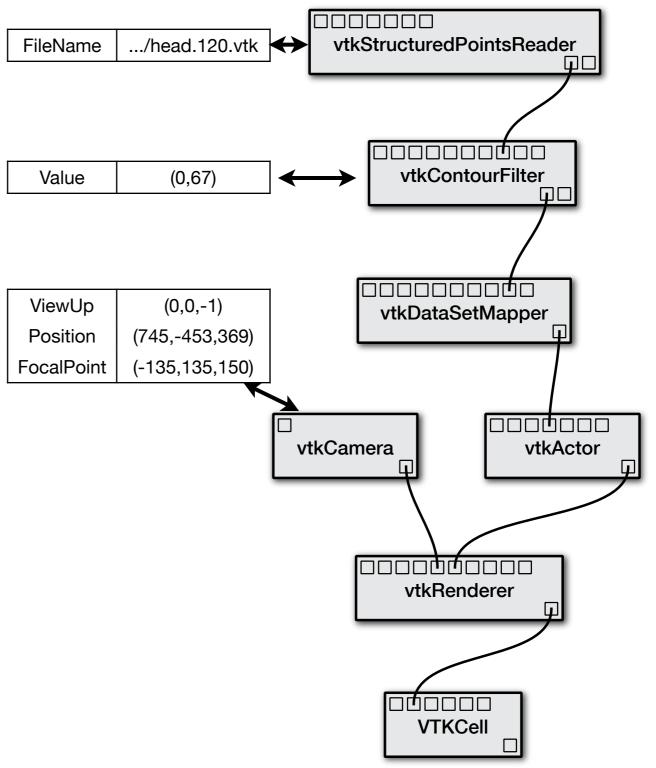
 Workflow- and process-based have better abstraction, OS-based requires minimal user effort once installed and can capture "hidden dependencies"

Provenance Granularity

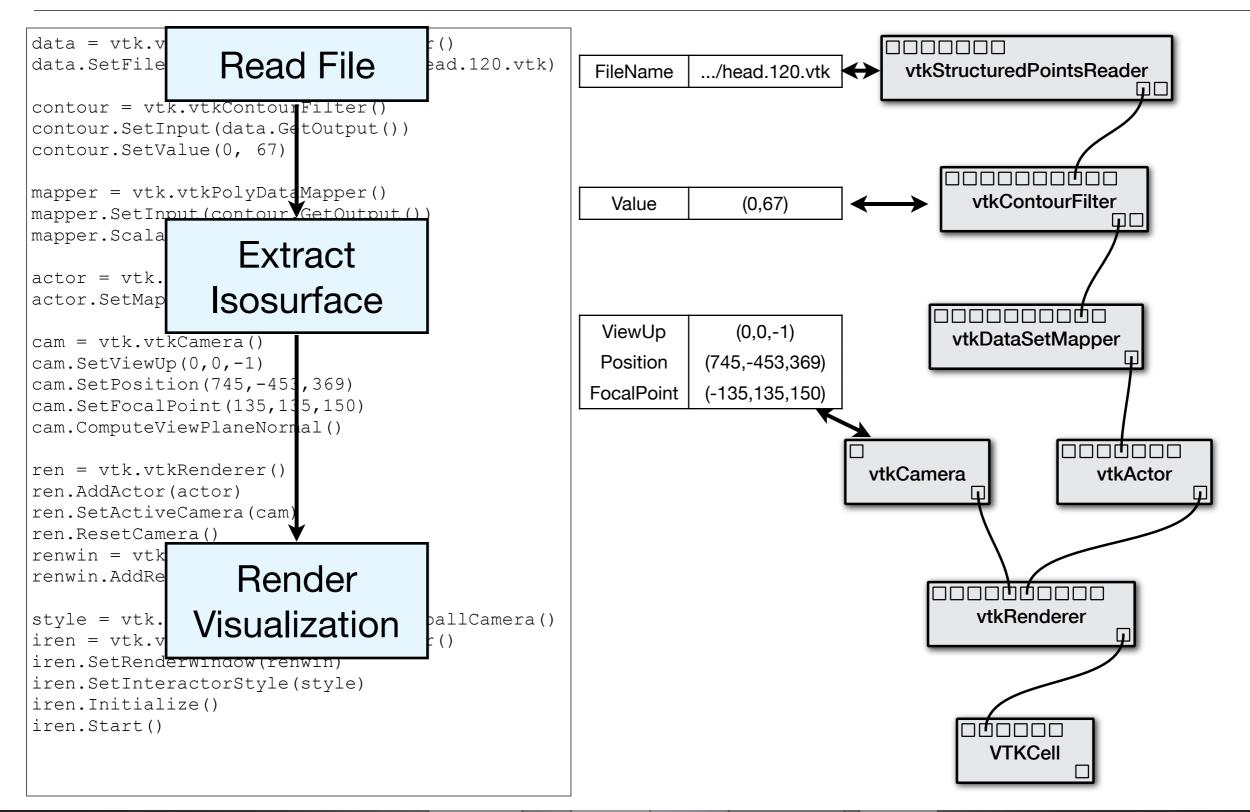
- How detailed should our provenance be?
 - Coarse: "This program ran with inputs x, y, z and produced outputs a, b, c"
 - Fine: "Input x was read into register 4, input y was read in register 5, add operation was performed using registers 4 and 5, ..."
- More queries are possible with fine-grained provenance, but...
 - Storage concerns
 - Performance concerns
- Abstraction can help here

Abstraction: Script, Workflow, Abstract Workflow

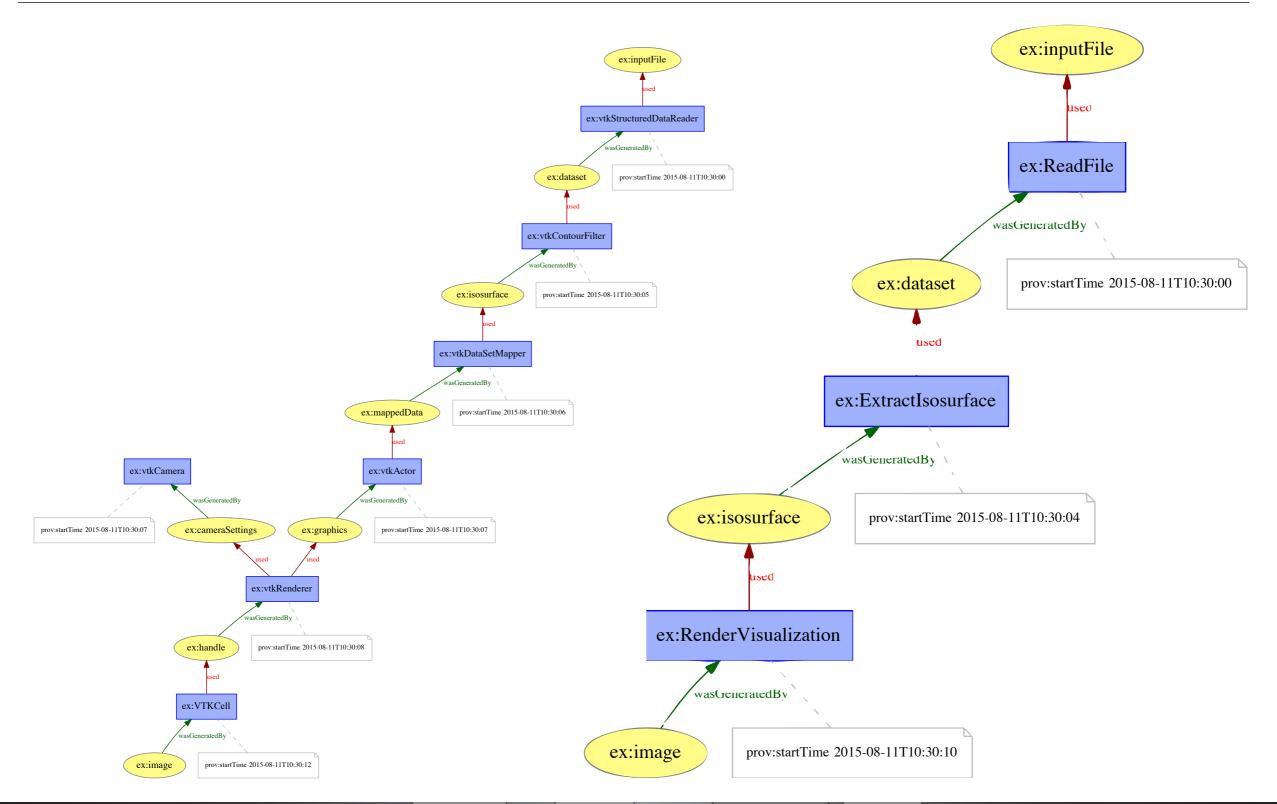
```
data = vtk.vtkStructuredPointsReader()
data.SetFileName(../examples/data/head.120.vtk)
contour = vtk.vtkContourFilter()
contour.SetInput(data.GetOutput())
contour.SetValue(0, 67)
mapper = vtk.vtkPolyDataMapper()
mapper.SetInput(contour.GetOutput())
mapper.ScalarVisibilityOff()
actor = vtk.vtkActor()
actor.SetMapper(mapper)
cam = vtk.vtkCamera()
cam.SetViewUp(0,0,-1)
cam. SetPosition (745, -453, 369)
cam.SetFocalPoint(135,135,150)
cam.ComputeViewPlaneNormal()
ren = vtk.vtkRenderer()
ren.AddActor(actor)
ren.SetActiveCamera(cam)
ren.ResetCamera()
renwin = vtk.vtkRenderWindow()
renwin.AddRenderer(ren)
style = vtk.vtkInteractorStyleTrackballCamera()
iren = vtk.vtkRenderWindowInteractor()
iren.SetRenderWindow(renwin)
iren.SetInteractorStyle(style)
iren.Initialize()
iren.Start()
```



Abstraction: Script, Workflow, Abstract Workflow



Abstraction: Provenance Views



Provenance Storage

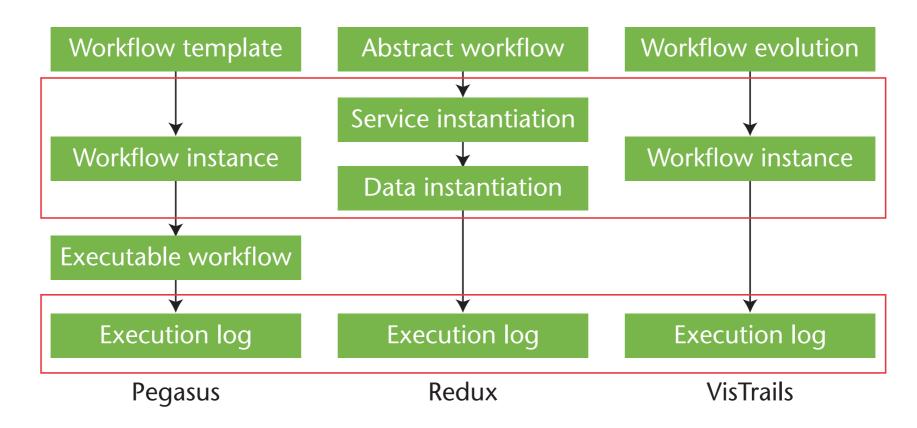
- Keeping provenance for each data item means lots of repetition
- Nested data storage also induces repetition
- Coarse provenance is naturally more compact, but how to decide what (not) to store?
- Repeated provenance is not uncommon:
 - Repeating the same computation with a different parameter
 - Creating a new computation that has a very similar structure to one that was run two weeks ago
- Provenance compression/factorization techniques (e.g. [Chapman et al., 2008], [Anand et al., 2009]) take advantage of that to reduce storage costs

Provenance Storage Formats

- Files, relational databases, XML databases, RDF (linked data)
- Log files are good for preserving data but can be bad to query or analyze
- Relational databases are great for column-specific queries but can be bad for dependency queries
- XML databases are more portable than relational databases but are usually less efficient for queries
- RDF triples are better for dependencies and integrating domainspecific knowledge but can be slower

Layered Provenance

- As with relational databases, want to normalize provenance to minimize redundant information
- Example: Don't store workflow specification each time that workflow is executed—store it once and reference it
- Also allow different layers for different aspects of provenance



Provenance Models

- How provenance is represented (more abstract than the details of how it is actually stored)
- PROV (W3C Standard) has different storage backends for provenance but all of it conforms to the same model
- Model the objects involved and their relationships (e.g. activities, dependencies)
- Interoperability is a concern
 - Why? May use multiple tools/techniques to achieve a result, want to analyze the entire provenance chain

Prospective and Retrospective Provenance

- Prospective provenance is what was specified/intended
 - a workflow, script, list of steps
- Retrospective provenance is what actually happened
 - actual data, actual parameters, errors that occurred, timestamps, machine information
- Do not need prospective provenance to have retrospective provenance!
- Retrospective provenance is often the same type of information as prospective plus more
- Could have multiple retrospective provenance traces for one prospective provenance listing

Prospective and Retrospective Provenance

- Example: Baking a Cake
- Prospective Provenance (Recipe):
 - 1. Gather ingredients (3/4 cup butter, 3/4 cocoa, 3/4 cup flour, ...)
 - 2. Preheat oven to 350 degrees
 - 3. Grease cake pan
 - 4. Mix wet ingredients in large bowl
 - 5. Mix dry ingredients in a separate bowl
 - 6. Add dry mixture to wet mixture
 - 7. Pour batter into cake pan
 - 8. Put pan in the oven and bake for 30 minutes
 - 9. Take cake out of oven and let it cool



Prospective and Retrospective Provenance

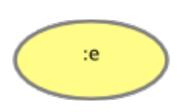
- Retrospective Provenance (What actually happened)
 - 1. Went to store to buy butter
- **\$**
- 2. Gathered ingredients (3/4 cup butter, 3/4 cocoa, 1 cup flour, ...)
- 3. Greased cake pan
- 4. Preheated oven to 350 degrees
- 5. Mixed wet ingredients in large bowl
- 6. Mixed dry ingredients in a separate bowl
- 7. Added wet mixture to dry mixture
- 8. Poured batter into cake pan
- 9. Put pan in the oven and baked for **35 minutes**
- 10. Took cake out of oven and let it cool for 10 minutes



Provenance Model History

- Community organized provenance challenges (2006-2009)
- First Provenance Challenge assessed capabilities of systems
- Second Provenance Challenge examined interoperability
- Led to development of Open Provenance Model (OPM), (2007)
 - Sought to establish interchange format for provenance
- Further work led to PROV W3C Recommendations (2013)
 - Some confusion from name changes from OPM to PROV even though concepts are similar
 - Focus is on **model** not formats

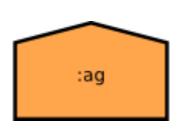
PROV: Three Key Classes



An **entity** is a physical, digital, conceptual, or other kind of thing with some fixed aspects; entities may be real or imaginary.



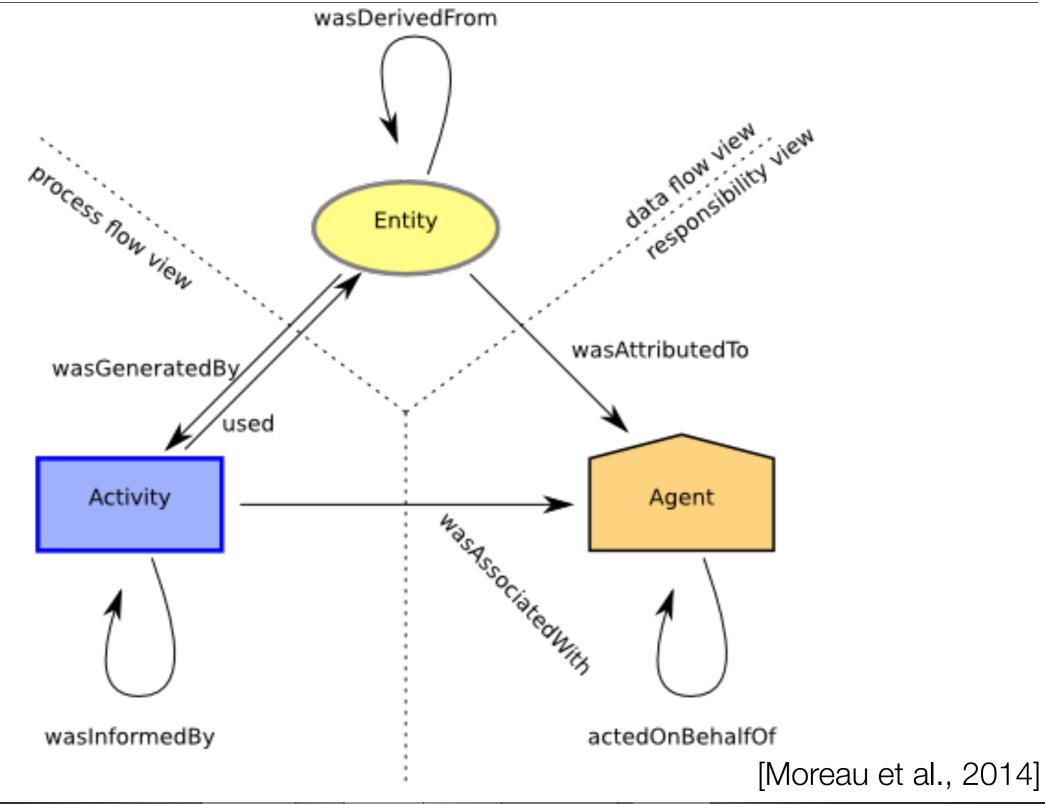
An **activity** is something that occurs over a period of time and acts upon or with entities; it may include consuming, processing, transforming, modifying, relocating, using, or generating entities.



An **agent** is something that bears some form of responsibility for an activity taking place, for the existence of an entity, or for another agent's activity.

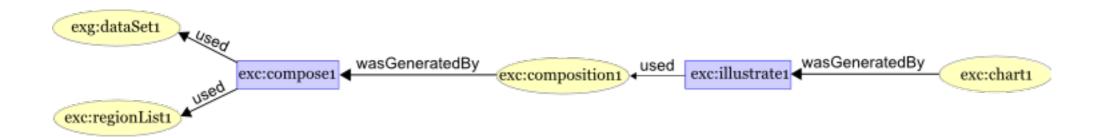
[Moreau et al., 2014]

PROV: Three Views of Provenance

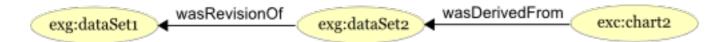


PROV Edges: Derivation

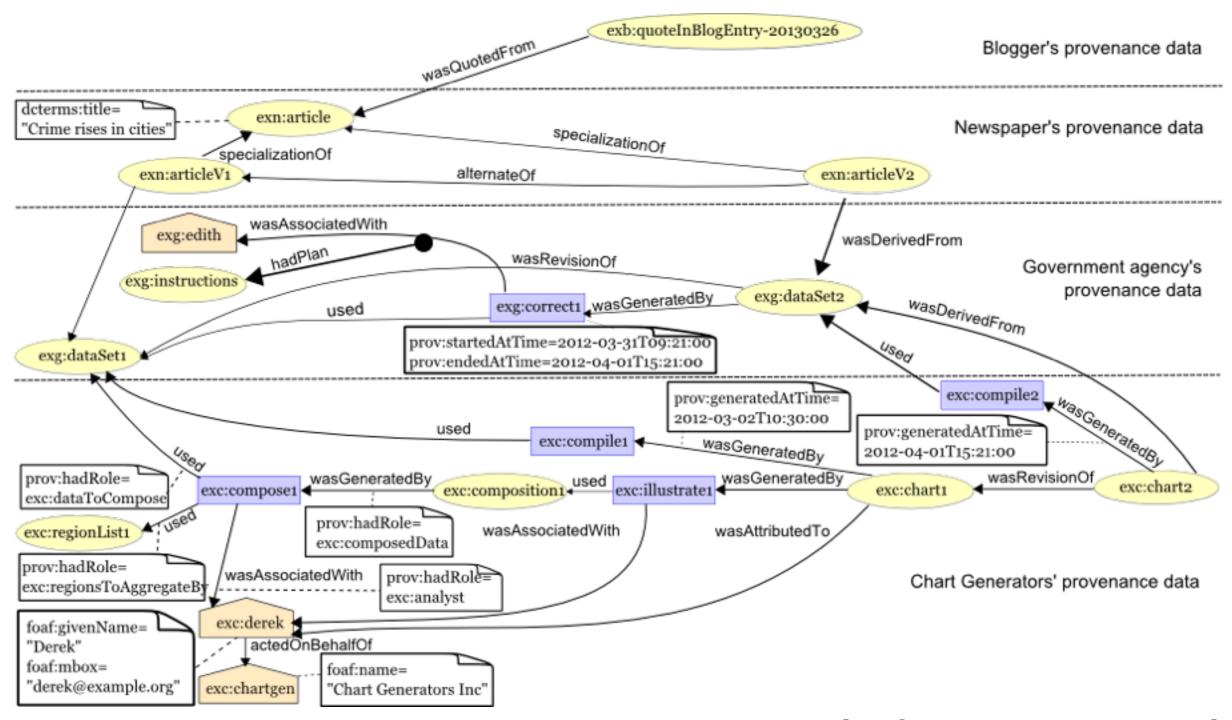
- Derivation Edges:
 - wasGeneratedBy: entity → activity
 - used: activity → entity



wasDerivedFrom: entity → entity



PROV Example



[PROV Model Primer, 2013]

Querying Provenance

- Query methods are often tied to storage backend
- SQL, XQuery, Prolog, SPARQL, ...

REDUX

```
SELECT Execution.ExecutableWorkflowId, Execution.ExecutionId, Event.EventId, ExecutableActivity.ExecutableActivityId from Execution_Event, Event, ExecutableWorkflow_ExecutableActivity, ExecutableActivity, ExecutableActivity_Property_Value, Value, EventType as ET where Execution.ExecutionId=Execution_Event.ExecutionId and Execution_Event.EventId=Event.EventId and ExecutableActivity.ExecutableActivityId=ExecutableActivity_Property_Value.ExecutableActivityId and ExecutableActivity_Property_Value.ValueId and Value.Value=Cast('-m 12' as binary) and ((CONVERT(DECIMAL, Event.Timestamp)+0)%7)=0 and Execution_Event.ExecutableWorkflow_ExecutableActivityId=ExecutableWorkflow_ExecutableActivity.ExecutableWorkflow_ExecutableActivityId and ExecutableWorkflow_ExecutableActivity.ExecutableWorkflowId=ExecutableActivity.ExecutableActivity.ExecutableActivityId=ExecutableActivity.ExecutableActivityId=ExecutableActivity.ExecutableActivityId=ExecutableActivity.ExecutableActivityId=ExecutableActivity.ExecutableActivityId=ExecutableActivity.ExecutableActivityId=ExecutableActivity.ExecutableActivityId=ExecutableActivity.ExecutableActivityId=ExecutableActivity.ExecutableActivityId=ExecutableActivity.ExecutableActivityId=ExecutableActivity.ExecutableActivityId=ExecutableActivity.ExecutableActivityId=ExecutableActivity.ExecutableActivityId=ExecutableActivity.ExecutableActivityId=ExecutableActivity.ExecutableActivityId=ExecutableActivity.ExecutableActivityId=ExecutableActivity.ExecutableActivityId=ExecutableActivity.ExecutableActivityId=ExecutableActivity.ExecutableActivityId=ExecutableActivity.ExecutableActivityId=ExecutableActivity.ExecutableActivityId=ExecutableActivity.ExecutableActivityId=ExecutableActivity.ExecutableActivityId=ExecutableActivity.ExecutableActivityId=ExecutableActivity.ExecutableActivityId=ExecutableActivity.ExecutableActivityId=ExecutableActivity.ExecutableActivityId=ExecutableActivity.ExecutableActivity.ExecutableActivity.ExecutableActivity.ExecutableActivity.ExecutableActivity.ExecutableActivity.ExecutableActivity.
```

VisTrails

wf{*}: x where x.module='AlignWarp' and x.parameter('model')='12' and (log{x}: y where y.dayOfWeek='Monday')

MyGrid

SELECT?p

where (?p <http://www.mygrid.org.uk/provenance#startTime> ?time) and (?time > date) using ns for <http://www.mygrid.org.uk/provenance#> xsd for <http://www.w3.org/2001/XMLSchema#>

SELECT ?p

where <urn:lsid:www.mygrid.org.uk:experimentinstance:HXQOVQA2ZI0>

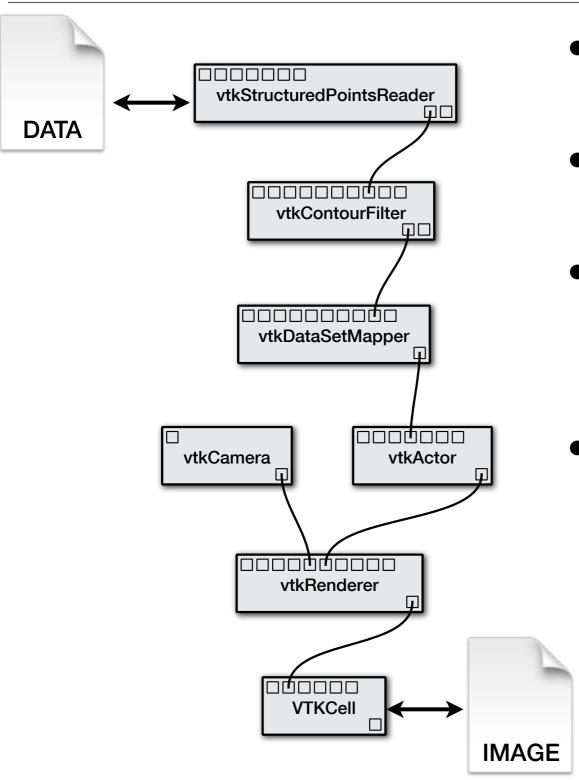
(?p <http://www.mygrid.org.uk/provenance#runsProcess> ?processname .

?p <http://www.mygrid.org.uk/provenance#processInput> ?inputParameter .

?inputParameter <ont:model> <ontology:twelfthOrder>)

using ns for http://www.mygrid.org.uk/ontology#>

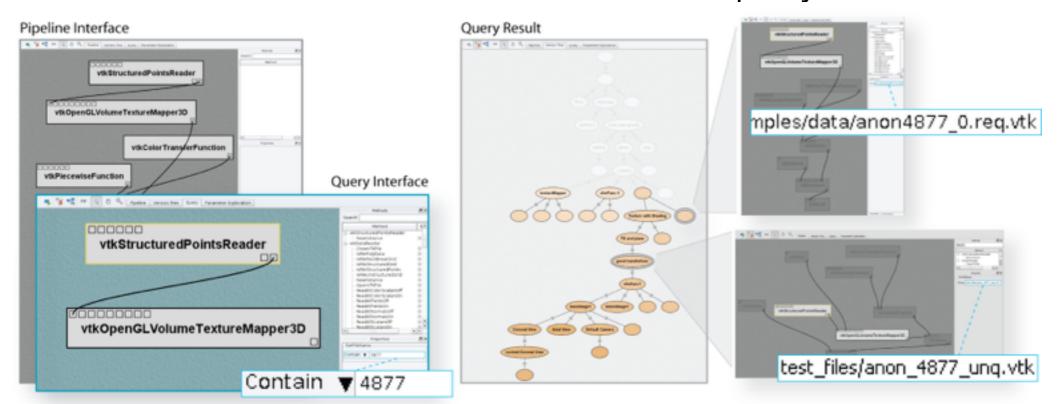
Querying Provenance



- What process led to the output image?
- What input datasets contributed to the output image?
- What workflows include resampling and isosurfacing with isovalue 57?
- Graph traversal or graph patterns
 - How do we write such queries?

Querying Provenance by Example

- Provenance is represented as graphs: hard to specify queries using text!
- Querying workflows by example [Scheidegger et al., TVCG 2007;
 Beeri et al., VLDB 2006; Beeri et al. VLDB 2007]
 - WYSIWYQ -- What You See Is What You Query
 - Interface to create workflow is same as to query



Stronger Links Between Provenance and Data

```
<workflow exec id="1">
 <m exec id="5"
          name="vtkStructuredDataReader"
          package="edu.utah.sci.vistrails.vtk"
          version="5.6.0">
    <param id="2" name="SetFile"</pre>
           value="/MyData/05-12-sc2.dat"/>
 </m exec>
 <m exec id="6"
          name="vtkContourFilter"
          package="edu.utah.sci.vistrails.vtk"
          version="5.6.0">
    <param id="3" name="SetValue"</pre>
           value="[1, 57]"/>
    <param id="4" name="ComputeScalarsOn"</pre>
           value="True"/>
 </m exec>
  <m exec id="11"
         name="FileSink"
         package="edu.utah.sci.vistrails.basic"
         version="1.5">
    <param id="15" name="path"</pre>
           value="/home/a/results/23.out"/>
 </m exec>
```

- Filenames are often the mode of identification in data exploration
- We might also use URIs or access curated data stores
 - Can this always be expected for exploratory tasks?
 - What happens if offline?
- Solution:
 - Managed store for data associated with computations
 - Improved data identification
 - Automatic versioning

Stronger Links Between Provenance and Data

```
<workflow exec id="1">
 <m exec id="5"
          name="vtkStructuredDataReader"
          package="edu.utah.sci.vist/_\ls.vtk"
          version="5.6.0">
   <param id="2" name="SetFile"</pre>
           value="/MyData/05-12-s
 </m exec>
                             FILE NOT FOUND
 <m exec id="6"
          name="vtkContourFilter"
          package="edu.utah.sci.vistrails.vtk"
          version="5.6.0">
    <param id="3" name="SetValue"</pre>
           value="[1, 57]"/>
    <param id="4" name="ComputeScalarsOn"</pre>
           value="True"/>
 </m exec>
 <m exec id="11"
         name="FileSink"
         package="edu.utah.sci.vistrails.basic"
         version="1.5">
    <param id="15" name="path"</pre>
           value="/home/a/results/23.out"/>
 </m exec>
```

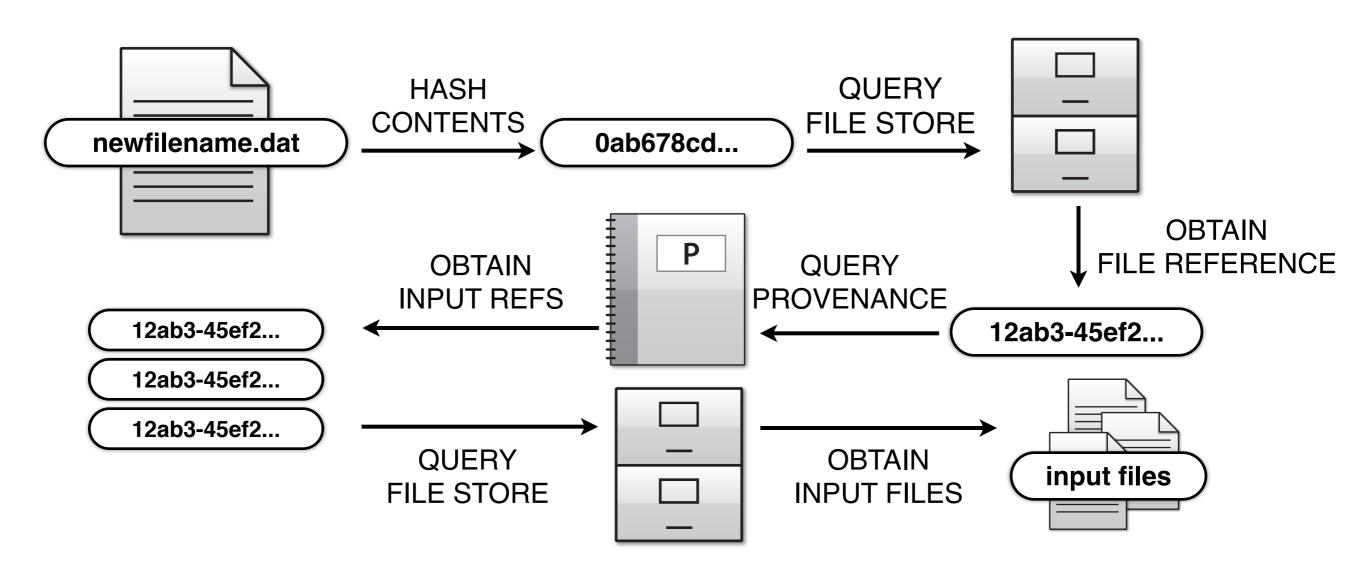
- Filenames are often the mode of identification in data exploration
- We might also use URIs or access curated data stores
 - Can this always be expected for exploratory tasks?
 - What happens if offline?
- Solution:
 - Managed store for data associated with computations
 - Improved data identification
 - Automatic versioning

Stronger Links Between Provenance and Data

```
<workflow exec id="1">
 <m exec id="5"
          name="vtkStructuredDataReader"
          package="edu.utah.sci.vist/_\ls.vtk"
          version="5.6.0">
    <param id="2" name="SetFile"</pre>
           value="/MyData/05-12-s
 </m exec>
                             FILE NOT FOUND
 <m exec id="6"
          name="vtkContourFilter"
          package="edu.utah.sci.vistrails.vtk"
          version="5.6.0">
    <param id="3" name="SetValue"</pre>
           value="[1, 57]"/>
    <param id="4" name="ComputeScalarsOn"</pre>
           value="True"/>
 </m exec>
 <m exec id="11"
         name="FileSink"
         package="edu.utah.sci.vistr/_\s.basic"
         version="1.5">
   <param id="15" name="path"</pre>
           value="/home/a/result
 </m exec>
                             FILE NOT FOUND
```

- Filenames are often the mode of identification in data exploration
- We might also use URIs or access curated data stores
 - Can this always be expected for exploratory tasks?
 - What happens if offline?
- Solution:
 - Managed store for data associated with computations
 - Improved data identification
 - Automatic versioning

Provenance from Data



Provenance-Enabled Systems

Table 1. Provenance-enabled systems.							
System	Capture mechanism	Prospective provenance	Retrospective provenance	Workflow evolution			
REDUX	Workflow-based	Relational	Relational	No			
Swift	Workflow-based	SwiftScript	Relational	No			
VisTrails	Workflow-based	XML and relational	Relational	Yes			
Karma	Workflow- and process-based	Business Process Execution Language	XML	No			
Kepler	Workflow-based	MoML	MoML variation	Under development			
Taverna	Workflow-based	Scufl	RDF	Under development			
Pegasus	Workflow-based	OWL	Relational	No			
PASS	OS-based	N/A	Relational	No			
ES3	OS-based	N/A	XML	No			
PASOA/PreServ	Process-based	N/A	XML	No			

Provenance-Enabled Systems

More...

Table 1. Provenanc						
System	Storage	Query support	Available as open source?			
REDUX	Relational database management system (RDBMS)	SQL	No			
Swift	RDBMS	SQL	Yes			
VisTrails	RDBMS and files	Visual query by example, specialized language	Yes			
Karma	RDBMS	Proprietary API	Yes			
Kepler	Files; RDBMS planned	Under development	Yes			
Taverna	RDBMS	SPARQL	Yes			
Pegasus	RDBMS	SPARQL for metadata and workflow; SQL for execution log	Yes			
PASS	Berkeley DB	nq (proprietary query tool)	No			
ES3	XML database	XQuery	No			
PASOA/PreServ	Filesystem, Berkeley DB	XQuery, Java query API	Yes			

Provenance-Enabled Systems



David Koop

Sumatra IPython Notebook More...

Table 1. Provenanc						
System	Storage	Query support	Available as open source?			
REDUX	Relational database management system (RDBMS)	SQL	No			
Swift	RDBMS	SQL	Yes			
VisTrails	RDBMS and files	Visual query by example, specialized language	Yes			
Karma	RDBMS	Proprietary API	Yes			
Kepler	Files; RDBMS planned	Under development	Yes			
Taverna	RDBMS	SPARQL	Yes			
Pegasus	RDBMS	SPARQL for metadata and workflow; SQL for execution log	Yes			
PASS	Berkeley DB	nq (proprietary query tool)	No			
ES3	XML database	XQuery	No			
PASOA/PreServ	Filesystem, Berkeley DB	XQuery, Java query API	Yes			

VisTrails



- Comprehensive provenance infrastructure for computational tasks
- Focus on exploratory tasks such as simulation, visualization, and data analysis
- Transparently tracks provenance of the discovery process—from data acquisition to visualization
 - The trail followed as users generate and test hypotheses
 - Users can refer back to any point along this trail at any time

ATPESC 2015

- Leverage provenance to streamline exploration
- Focus on usability—build tools for scientists

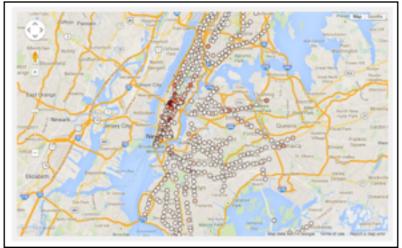
VisTrails

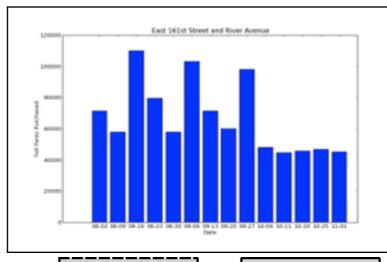


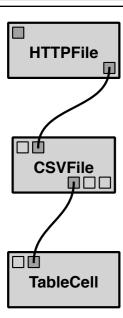
- Open-source, freely downloadable system (<u>www.vistrails.org</u>)
 - Also on GitHub (github.com/vistrails), PyPI, conda package
- Multi-platform: users on Mac, Linux, and Windows
- Python code and uses PyQt and Qt for the interface
- Over 35,000 downloads
- User's guide, wiki, and mailing list
- Many users in different disciplines and countries:
 - Visualizing environmental simulations (CMOP STC)
 - Simulation for solid, fluid and structural mechanics (Galileo Network, UFRJ Brazil)
 - Quantum physics simulations (ALPS, ETH Zurich)
 - Climate analysis (UV-CDAT, LLNL)
 - Habitat modeling (USGS)
 - Open Wildland Fire Modeling (U. Colorado, NCAR)
 - High-energy physics (LEPP, Cornell)
 - Cosmology simulations (LANL)

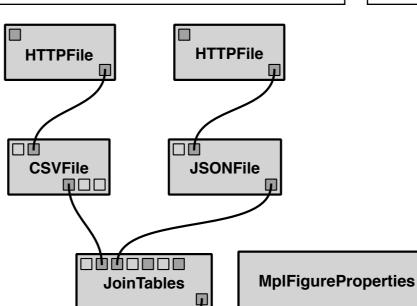
- Using tms for improving memory (Pyschiatry, U. Utah)
- eBird (Cornell, NSF DataONE)
- Astrophysical Systems (LSU)
- NIH NBCR (UCSD)
- Pervasive Technology Labs (Indiana University)
- Linköping University
- University of North Carolina, Chapel Hill
- UTEP

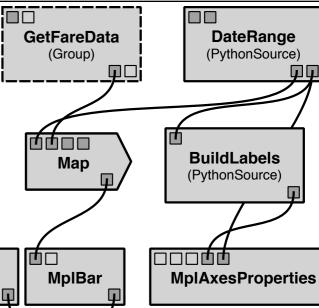












Parameters

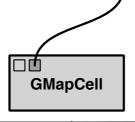
HTTPFile.url web.mta.info/.../fares_130824.csv

CSVFile.skip_lines 2

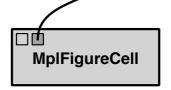
JoinTables.left_col STATION

JoinTables.right_col __key

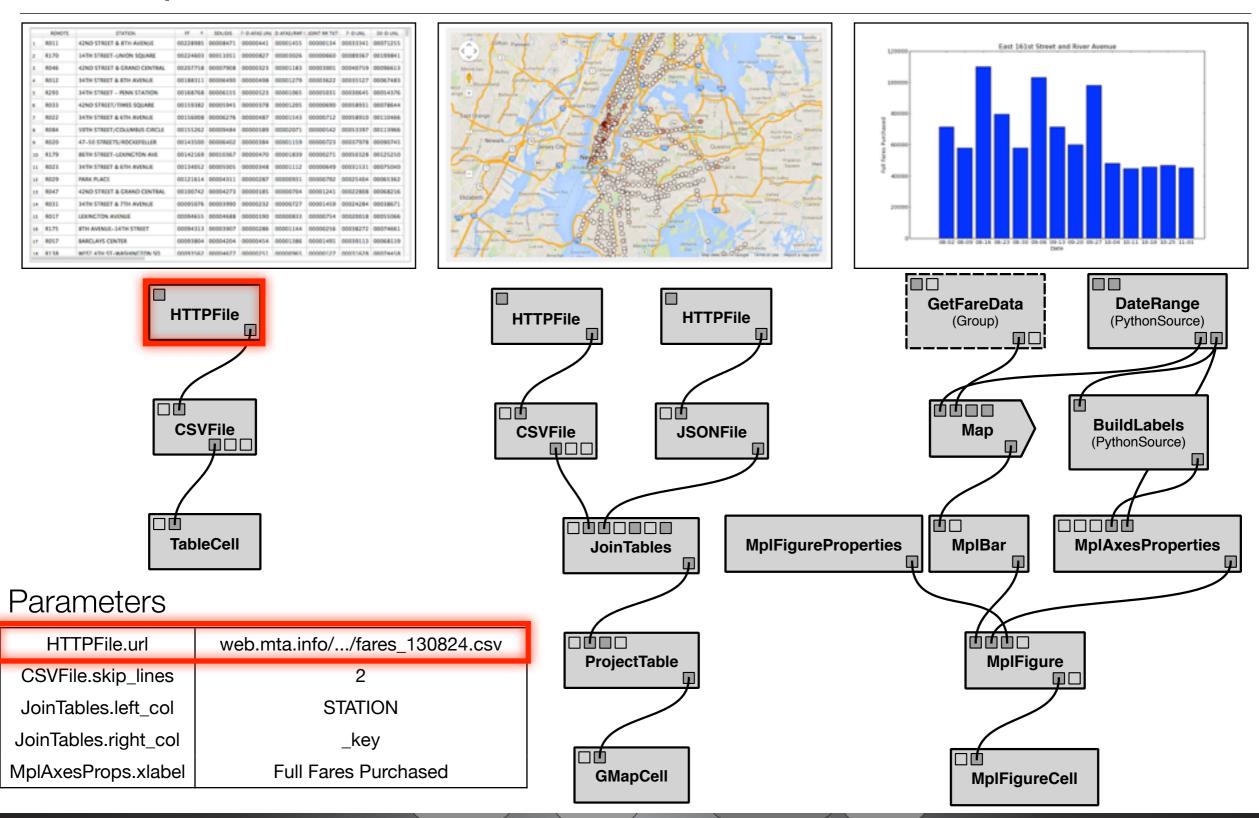
MplAxesProps.xlabel Full Fares Purchased

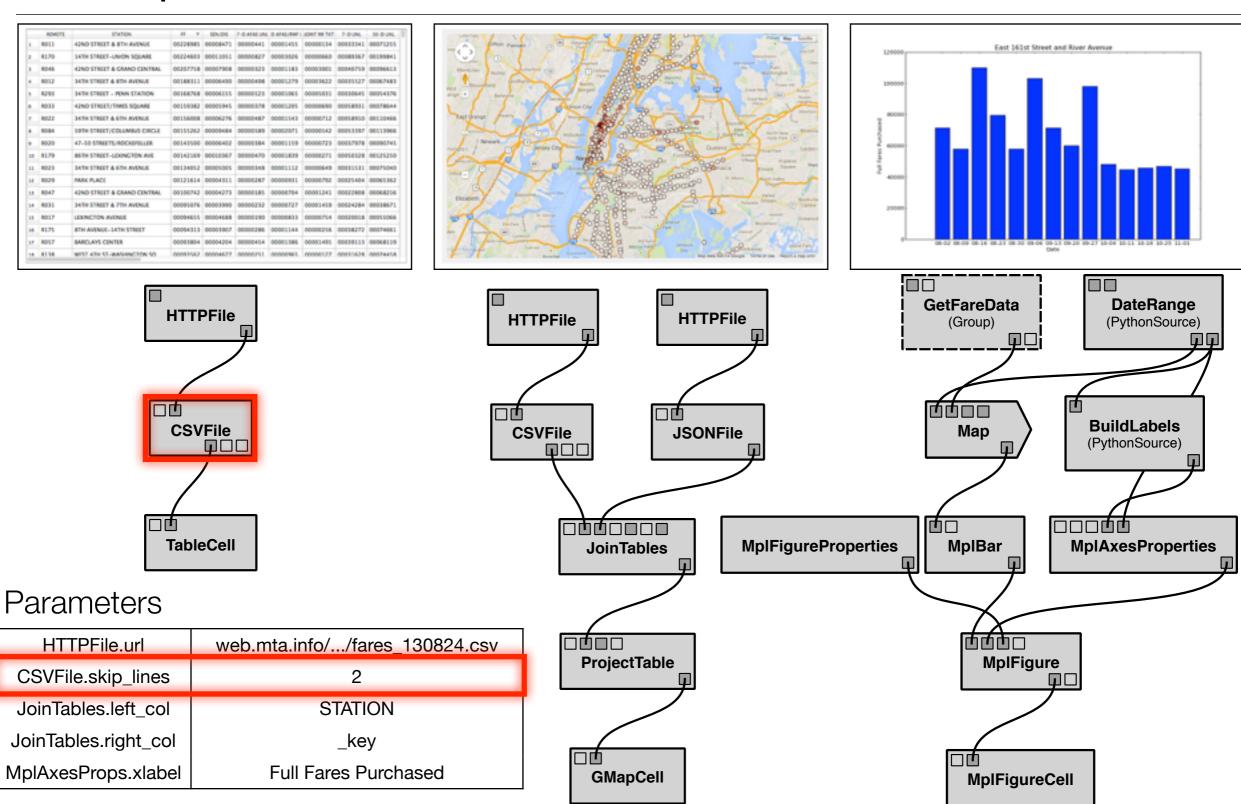


ProjectTable

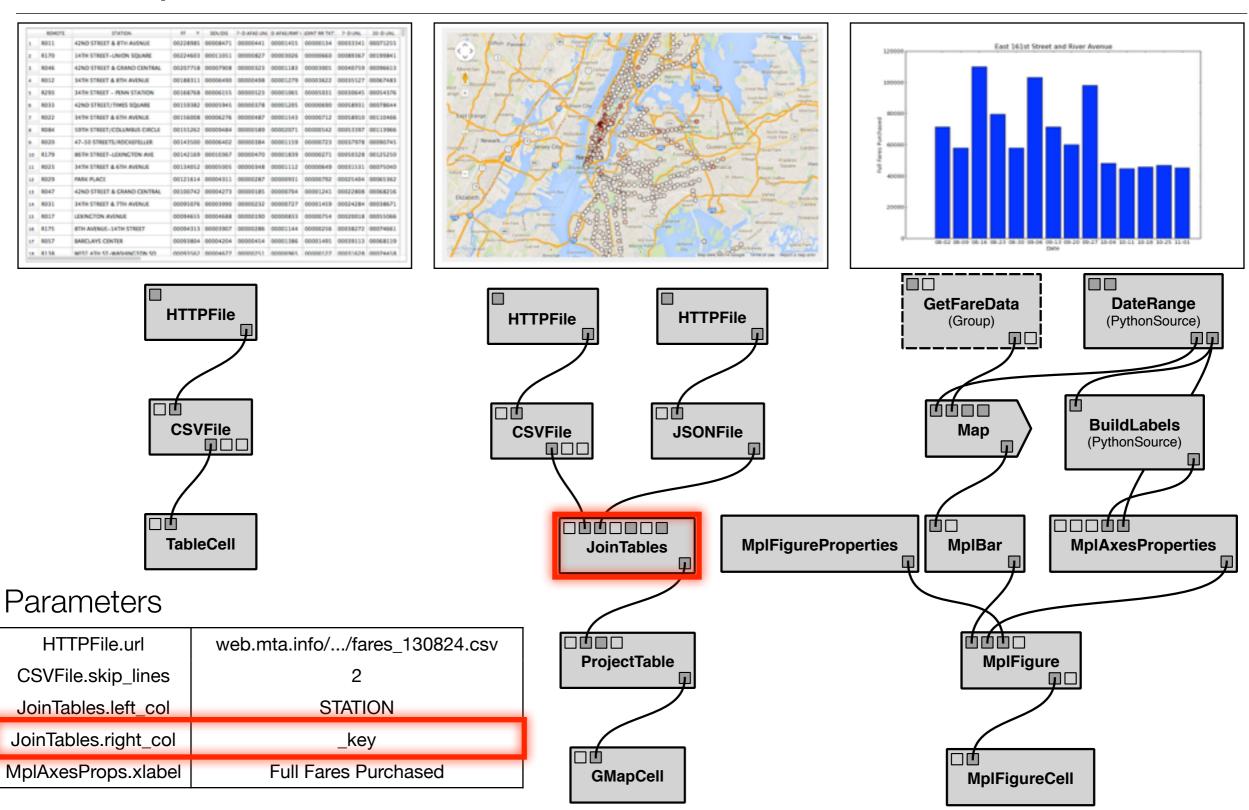


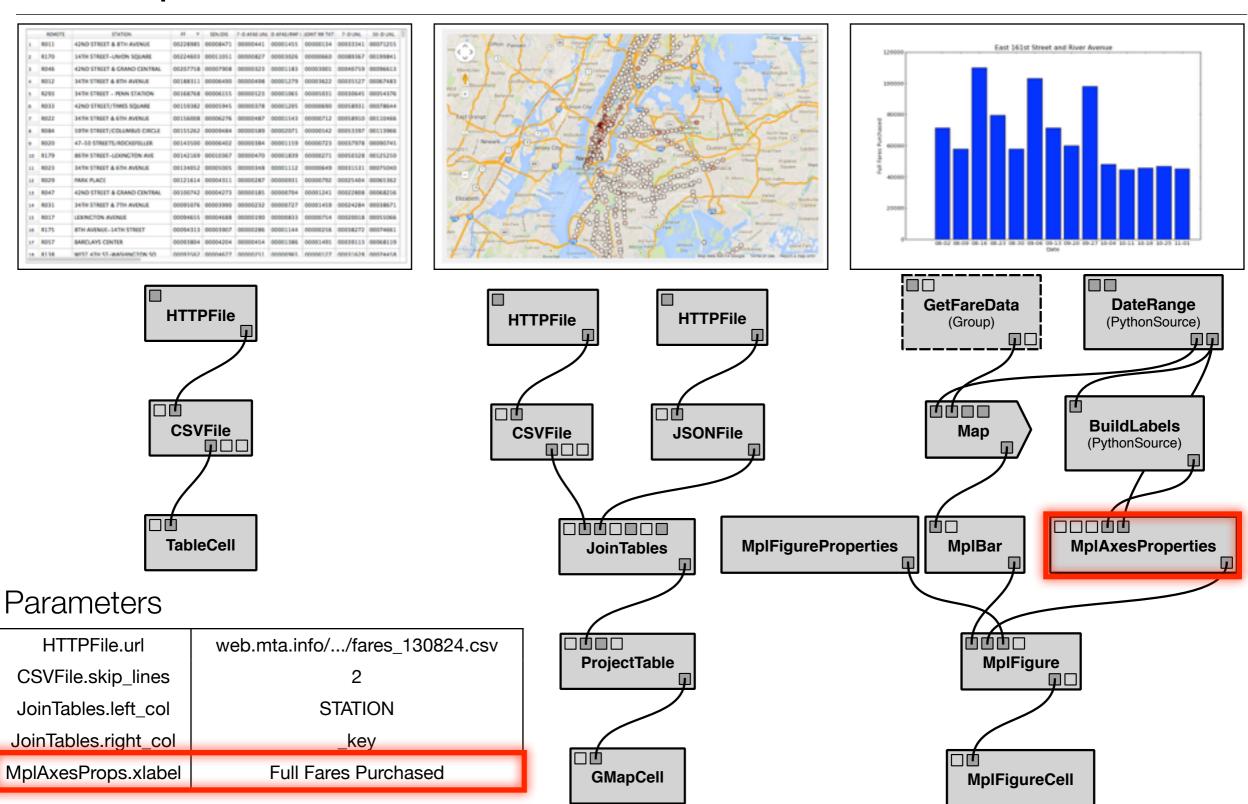
MplFigure



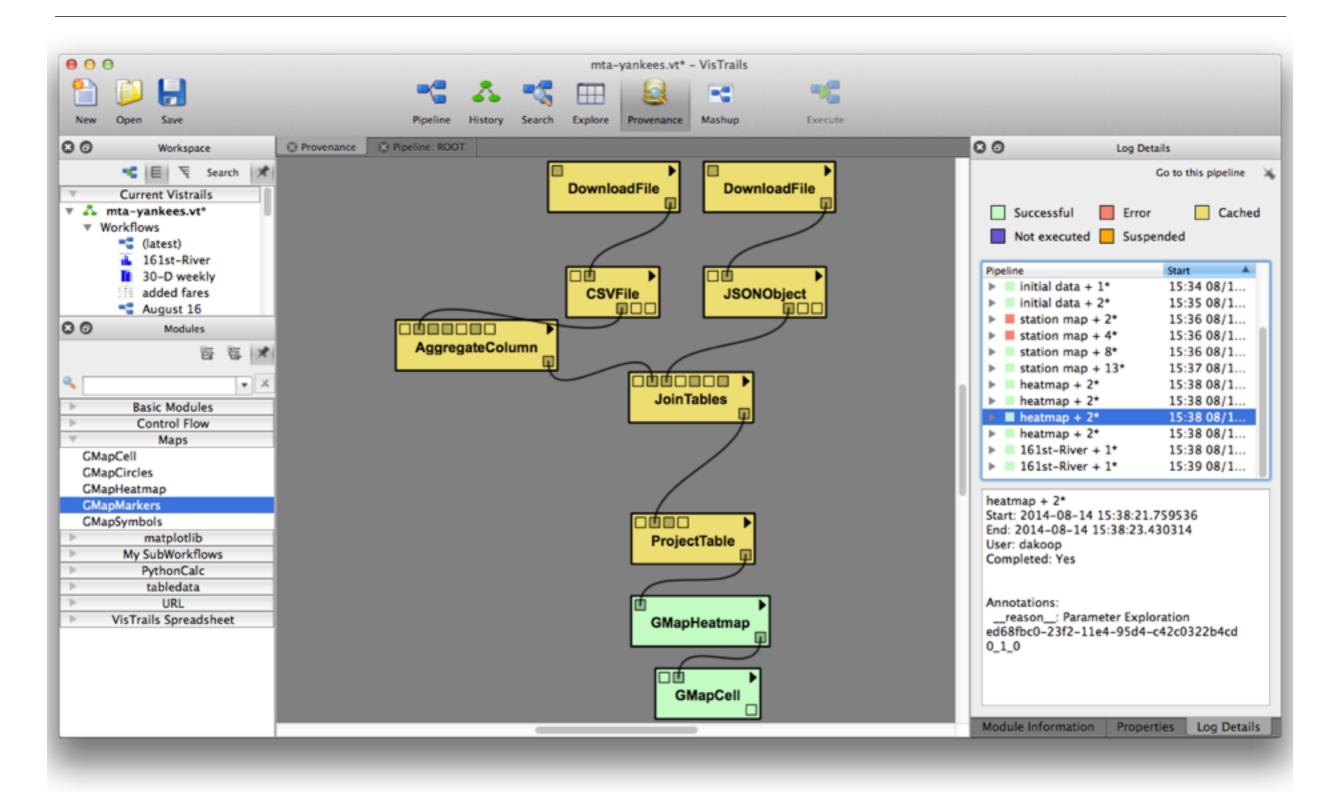




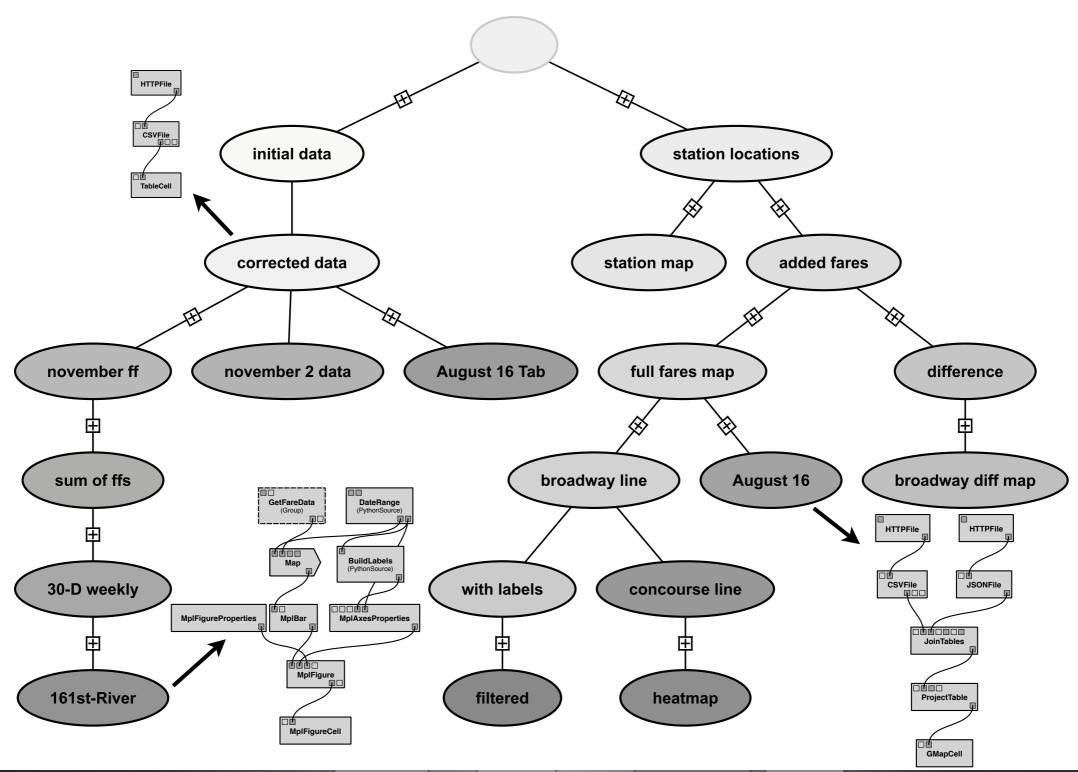


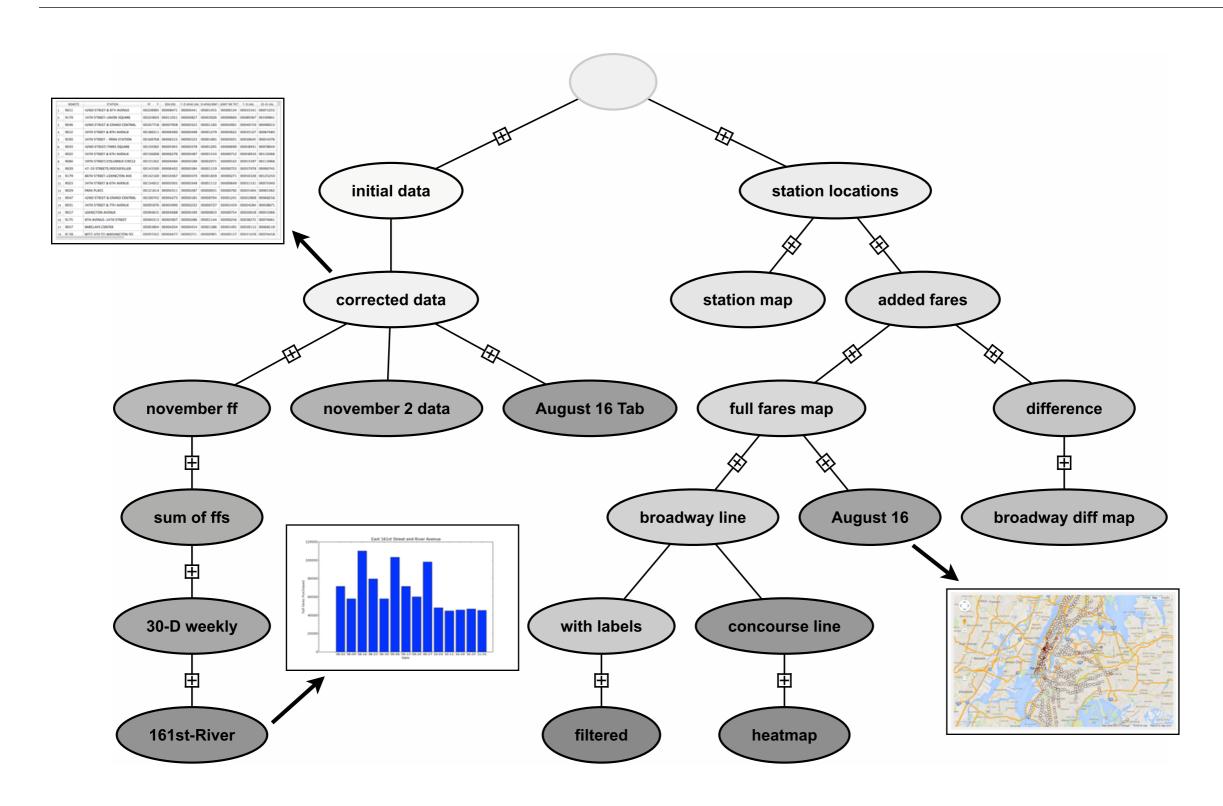


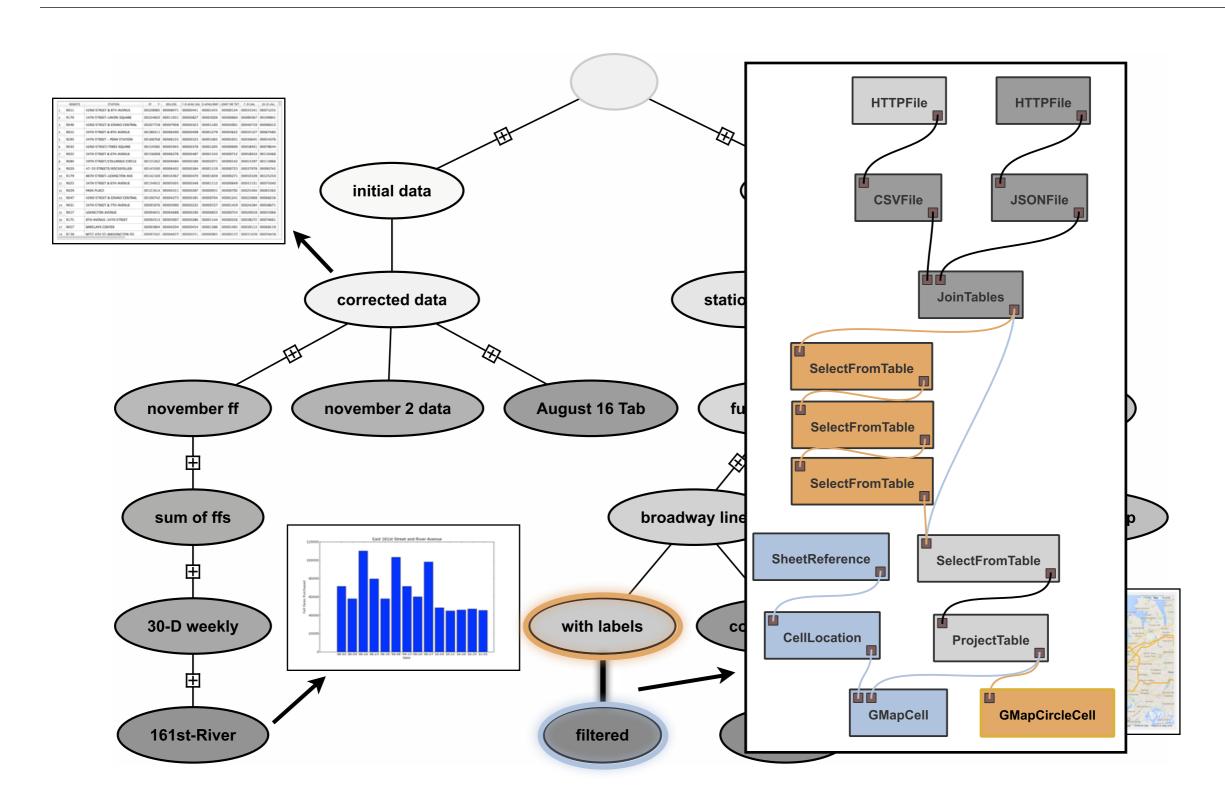
Execution Provenance

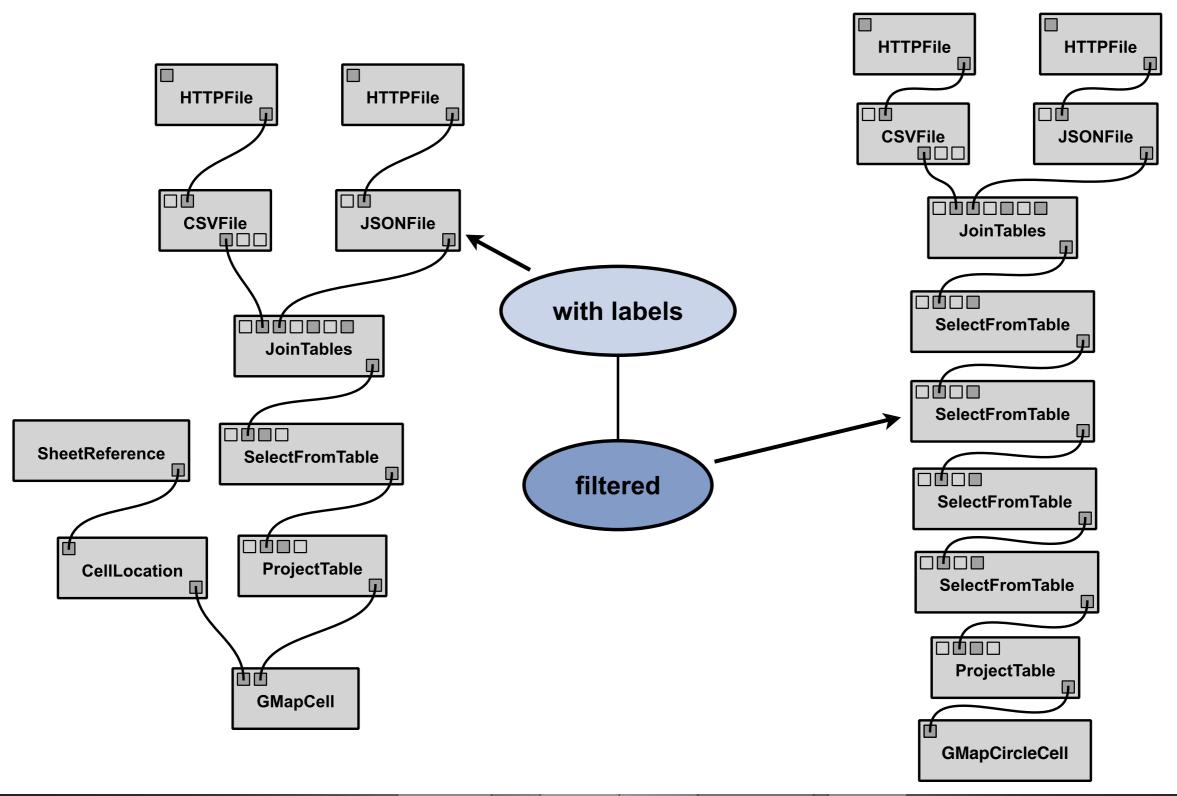


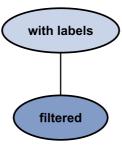
Workflow Evolution Provenance

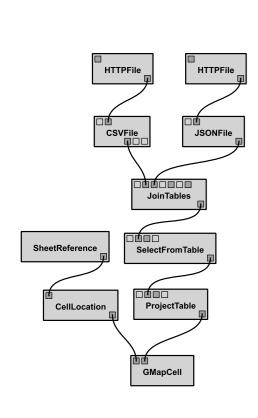






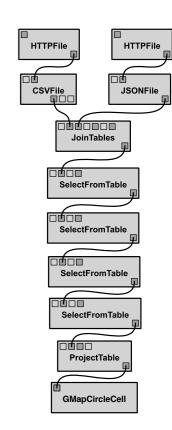




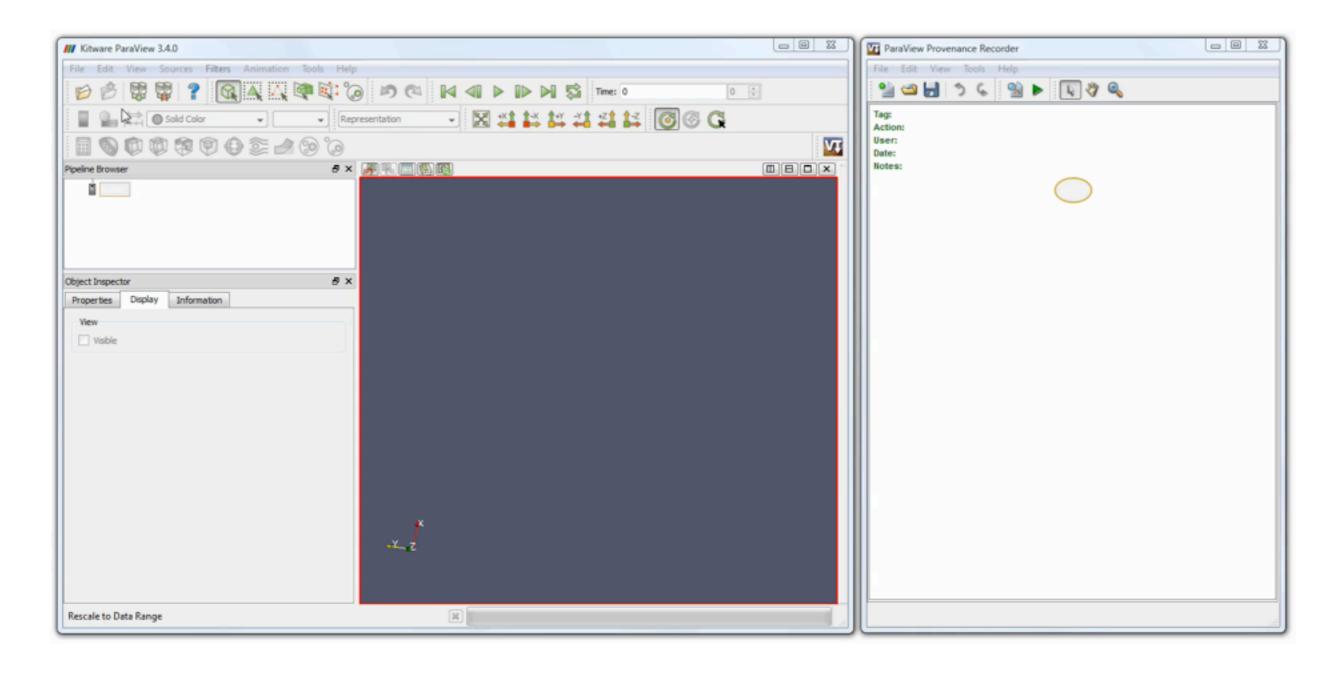


delete module "GMapCell"
delete module "CellLocation"
delete module "ProjectTable"
delete module "SelectFromTable"

add module "SelectFromTable"
add parameter "float_expr" to "SelectFromTable" with value "latitutde > 40.6"
delete parameter "float_expr" from "SelectFromTable"
add parameter "float_expr" to "SelectFromTable" with value "latitutde > 40.7"
delete parameter "float_expr" from "SelectFromTable"
add parameter "float_expr" to "SelectFromTable" with value "latitutde > 40.8"

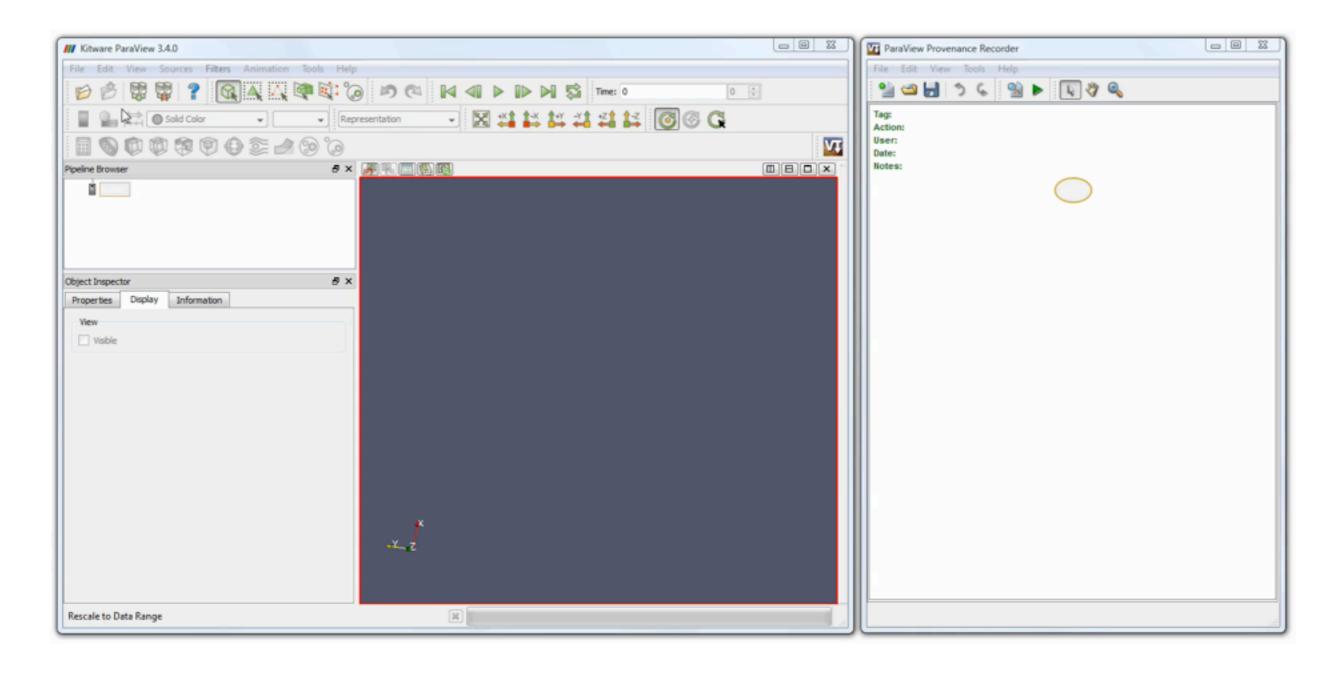


Evolution Provenance for ParaView



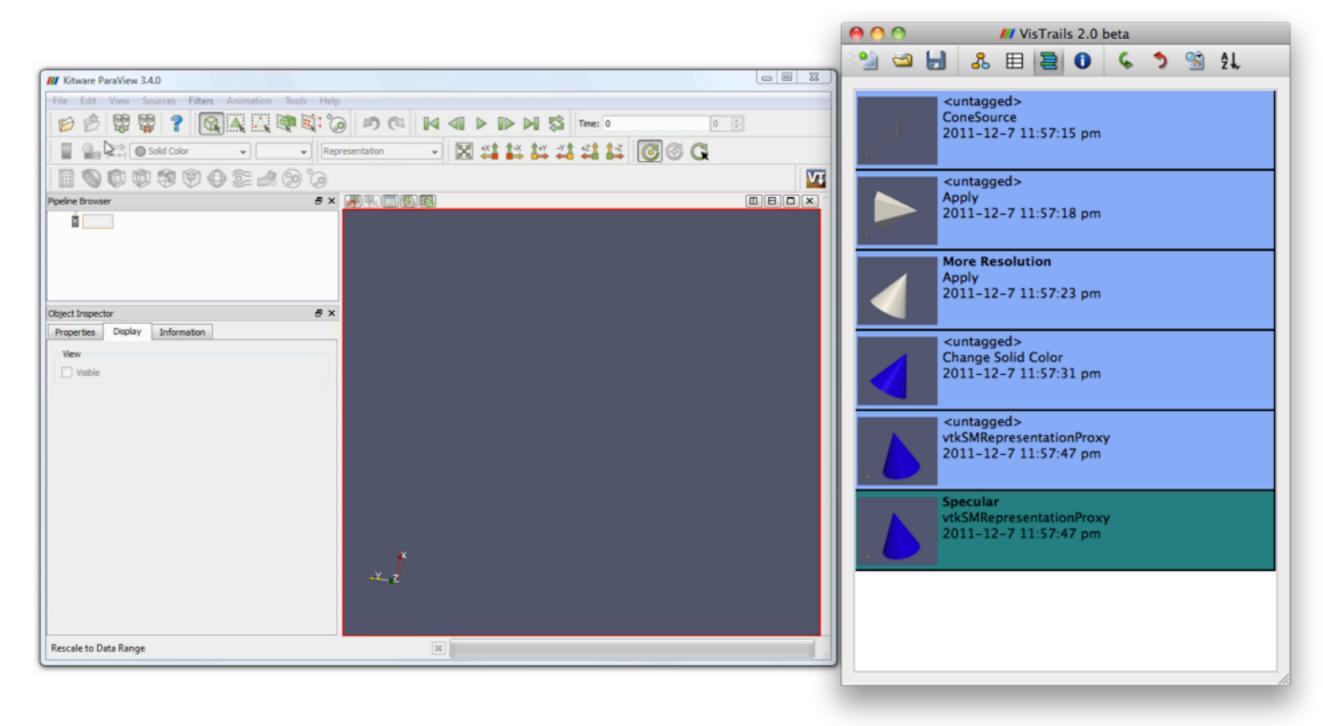
[VisTrails, Inc.]

Evolution Provenance for ParaView



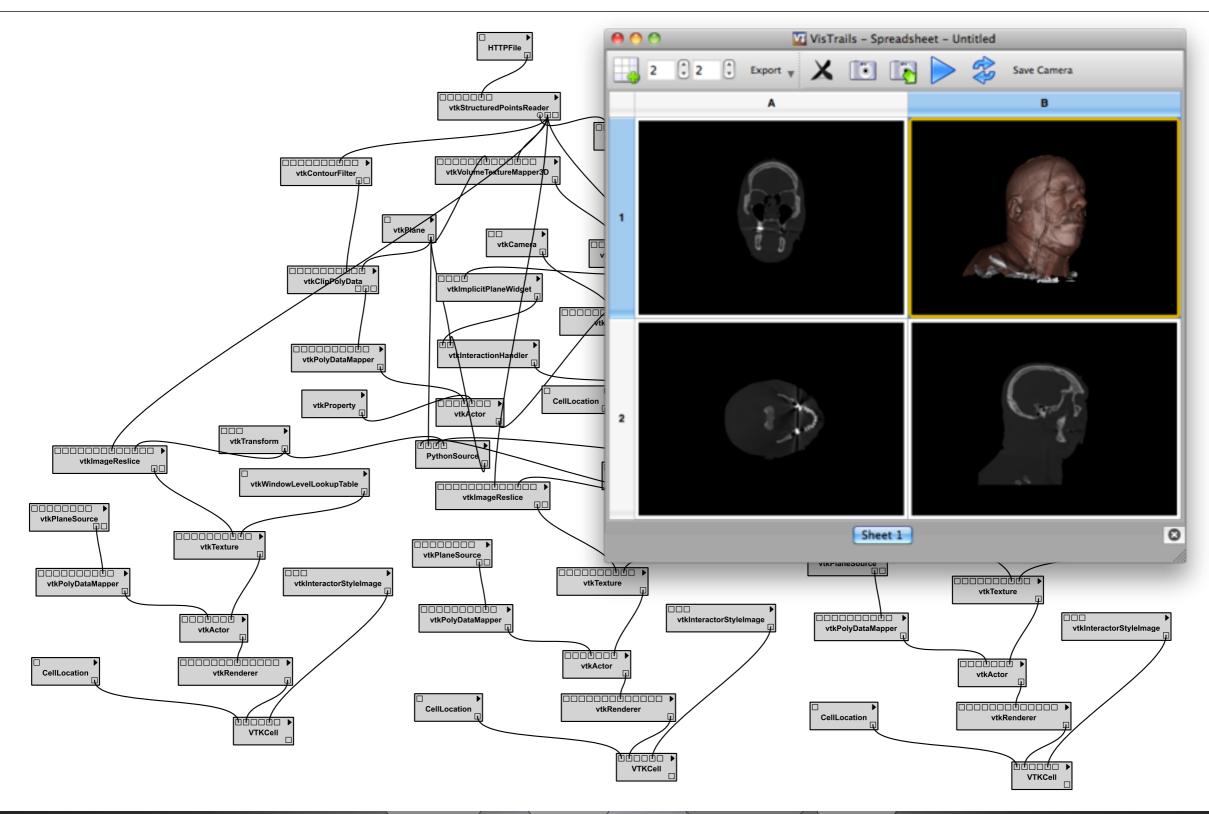
[VisTrails, Inc.]

Evolution Provenance for ParaView

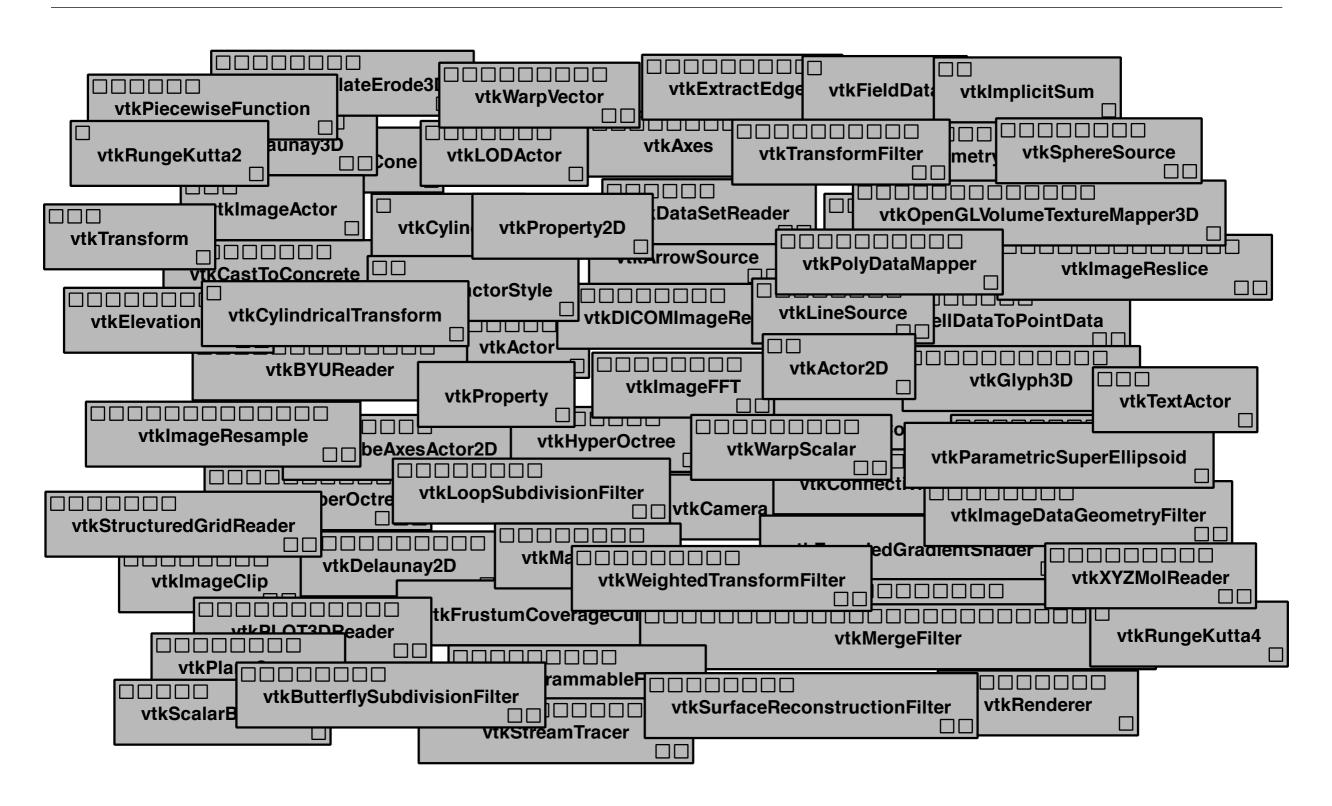


[VisTrails, Inc.]

Building Visualization Pipelines



Building Visualization Pipelines



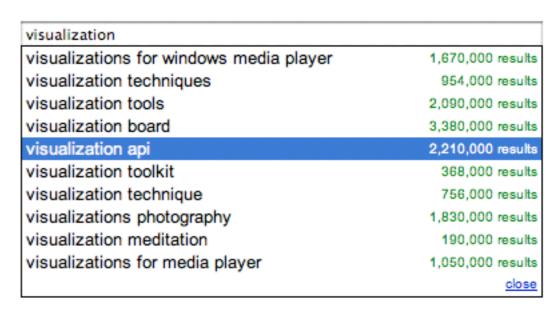
Completions

```
en.wikipedia.org/
http://en.wikipedia.org/
http://encarta.msn.com/
http://www.engadget.com/
http://www.engadget.com/2008/09/09/live-from-apples-lets-rock-event-in-san-francisco/
http://en.wikipedia.org/wiki/VisTrails
http://en.wikipedia.org/wiki/ACM_Transactions_on_Graphics
http://en.wikipedia.org/wiki/Barack_Obama
http://en.wikipedia.org/wiki/Columbus,_Ohio
http://en.wikipedia.org/wiki/Joe_Biden
http://en.wikipedia.org/wiki/John_McCain
```

[URL Completion, Safari]

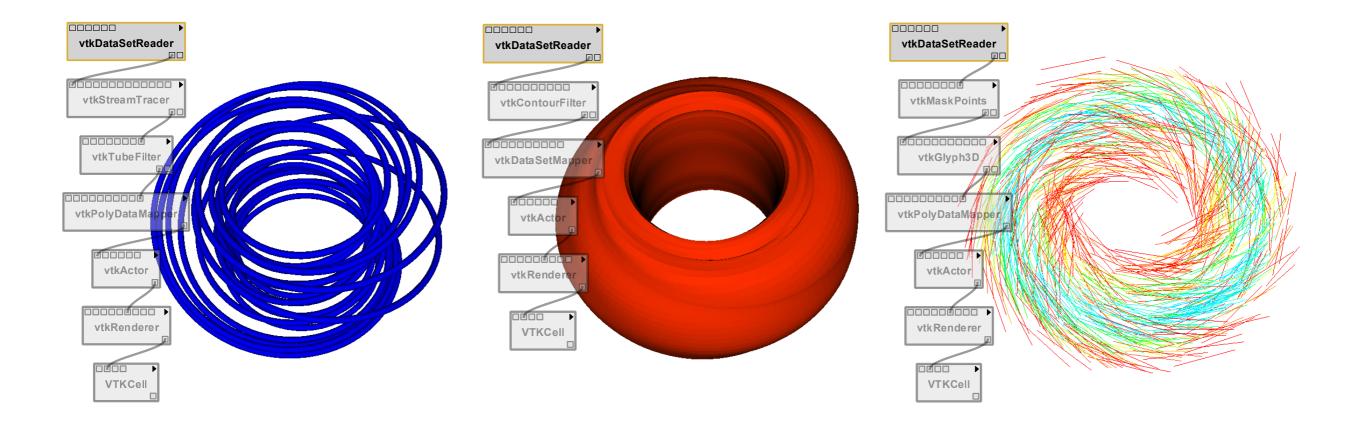
```
PowerPoint.Shape pic = sld.Shapes.
       20, 20, 128, 128, "multiple
                                        🗐 AddDiagram
                                                             nv
  //PowerPoint.Shape pic = Global AddLabel
                                                           icat
         "d:/hvo/vgc/src/vistrails → AddLine
                                                           /gui
         Microsoft.Office.Core.Mso | ■ AddMediaObject
                                         AddOLEObject
lidth, float Height, string ClassName, string FileName,
nLabel, Microsoft.Office.Core.MsoTriState Link)
                                         AddPicture
                                         AddPlaceholder
  //System.Diagnostics.Process.St
                                                           /pvt
                                         AddPolyline
          "d:/hvo/vgc/src/vistrails
                                                           /vis
                                         AddShape
                                         AddTable
```

[Code Completion, Intellisense]



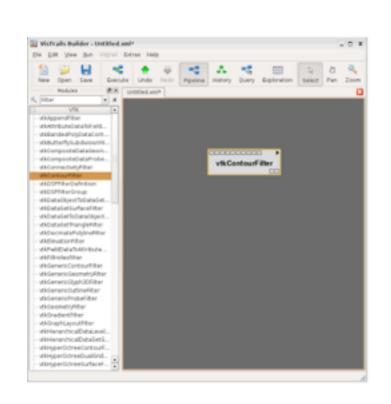
[Web Search Completion, Google]

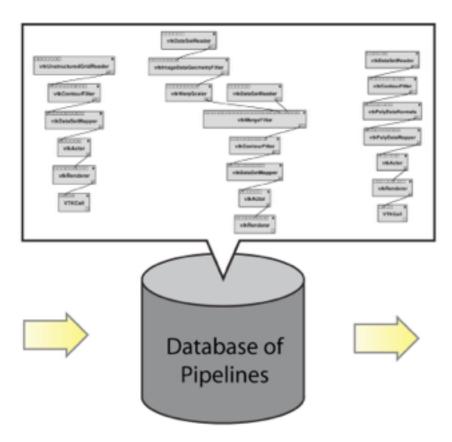
Visualization Pipeline Completions



VisComplete Overview

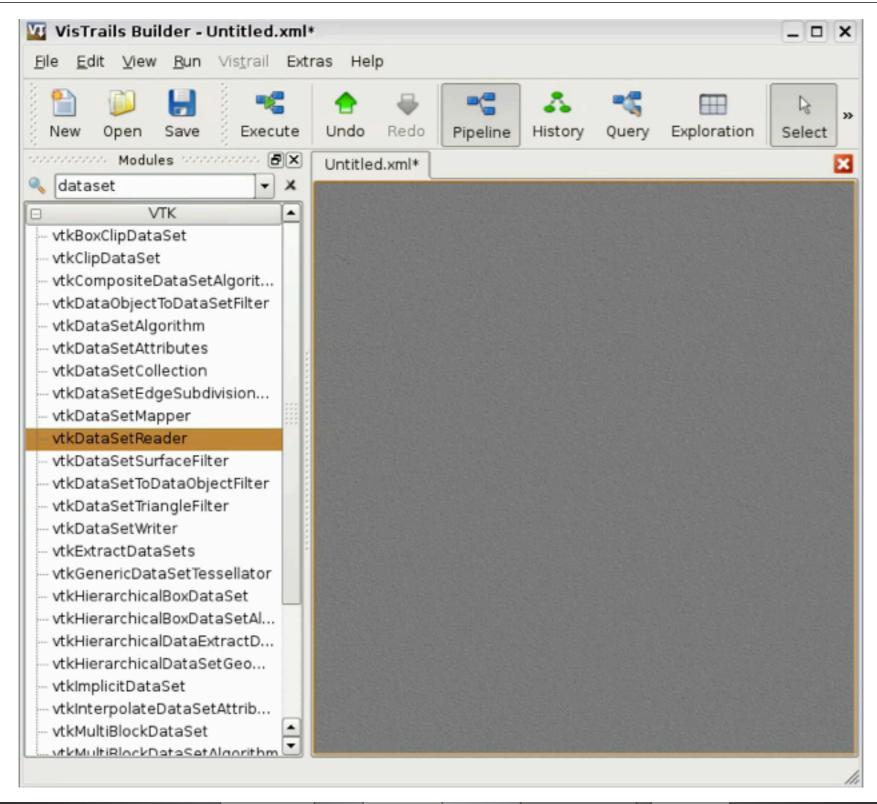
- Mine provenance collection: Identify graph fragments that co-occur in a collection of workflows (Data-Driven)
- Predict sets of likely workflow additions to a given partial workflow



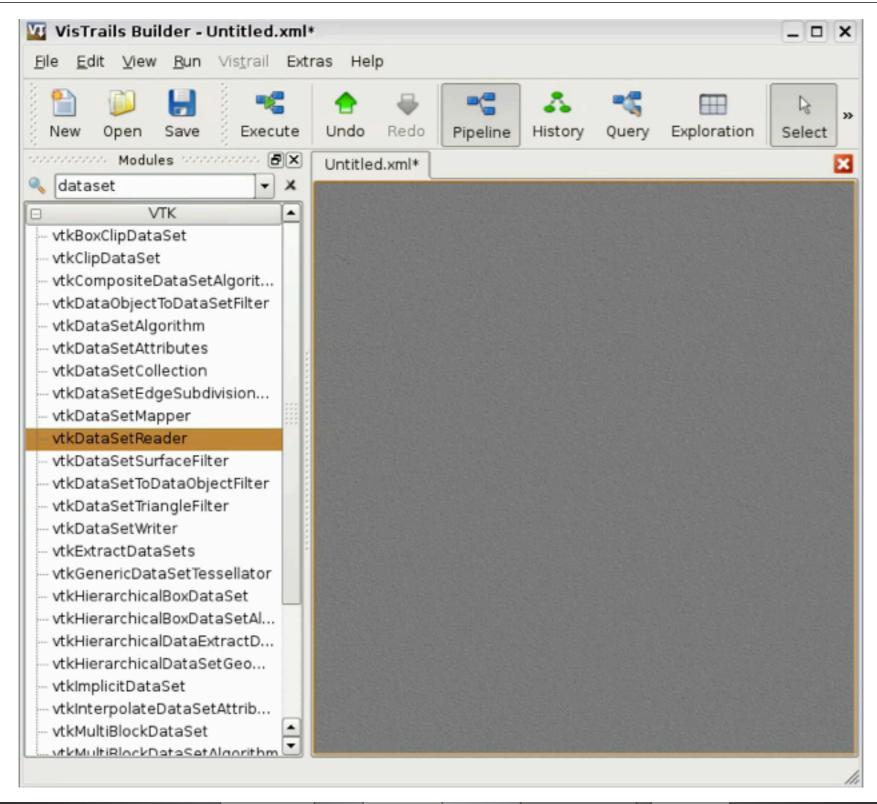




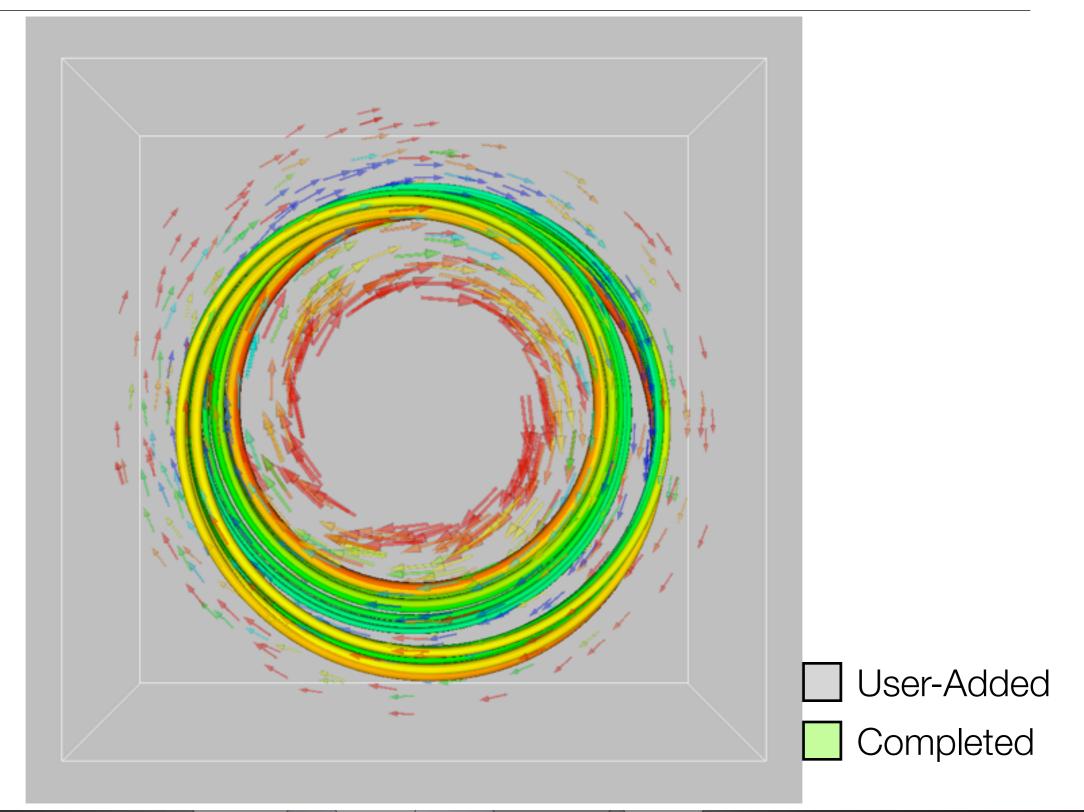
Suggestion Interface



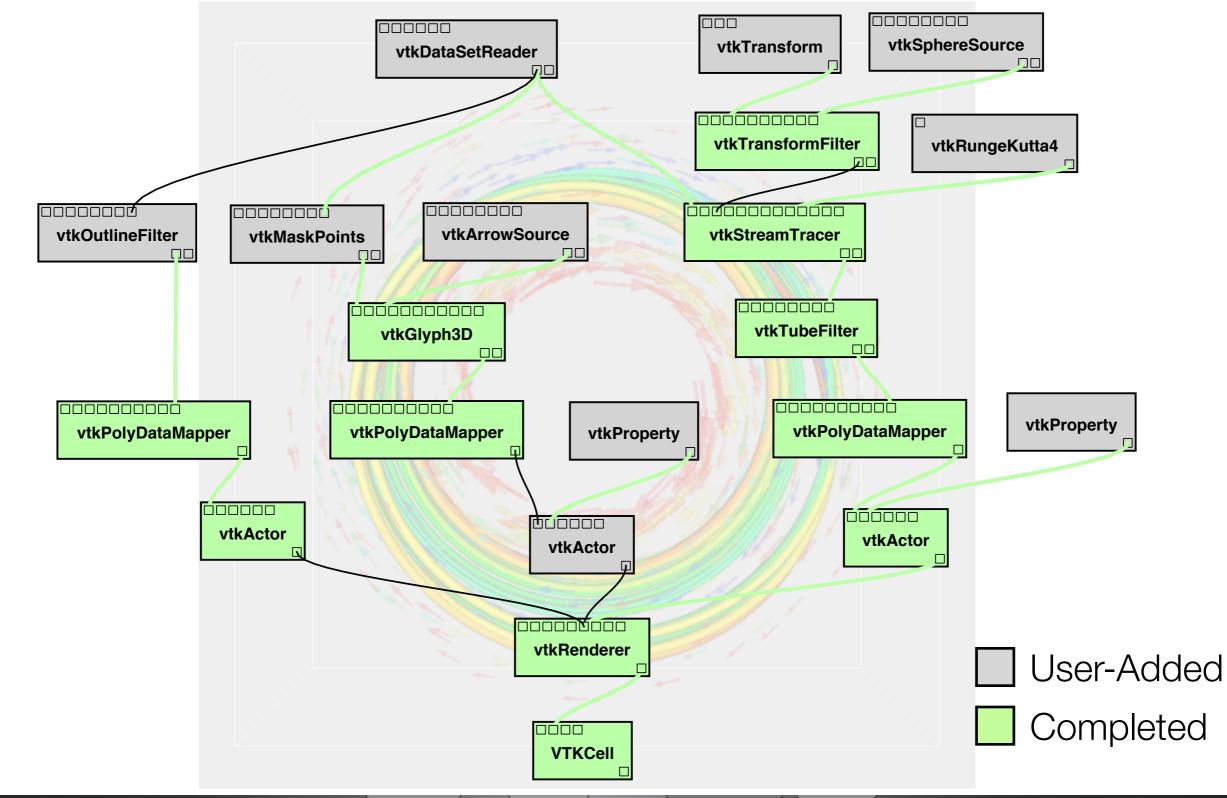
Suggestion Interface

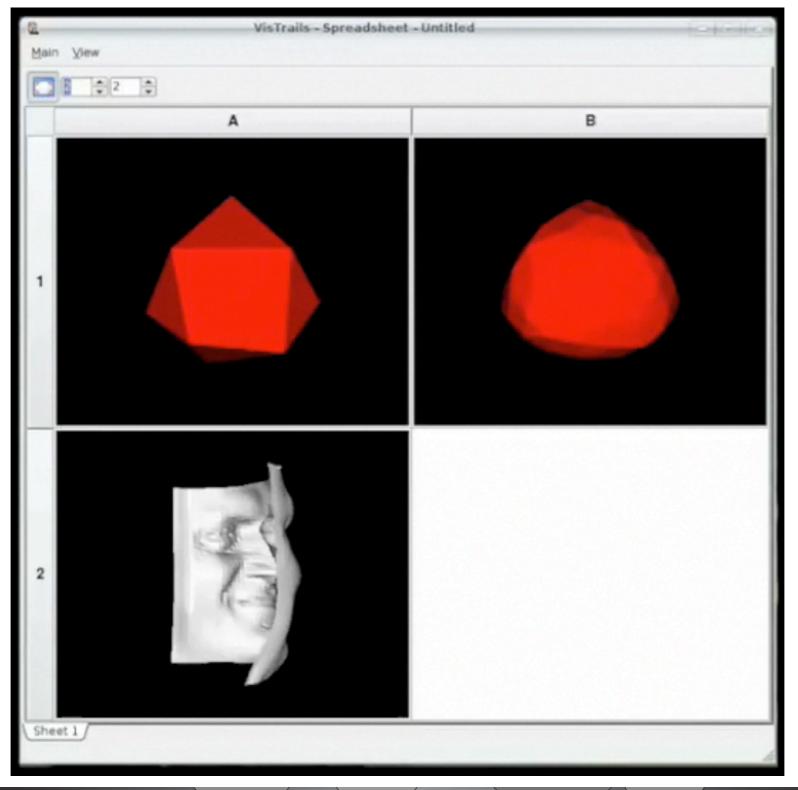


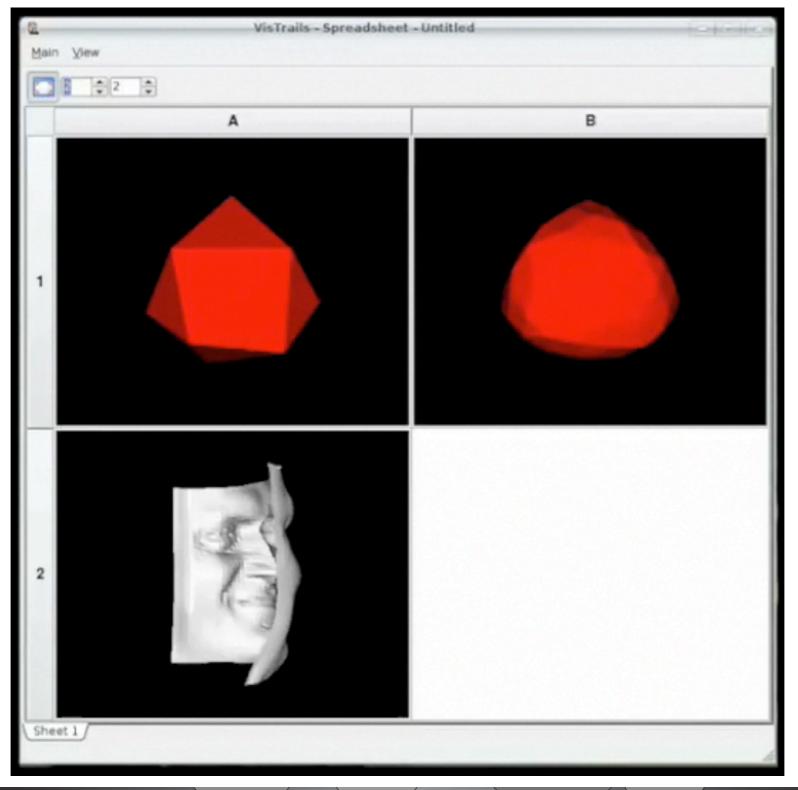
VisComplete Results

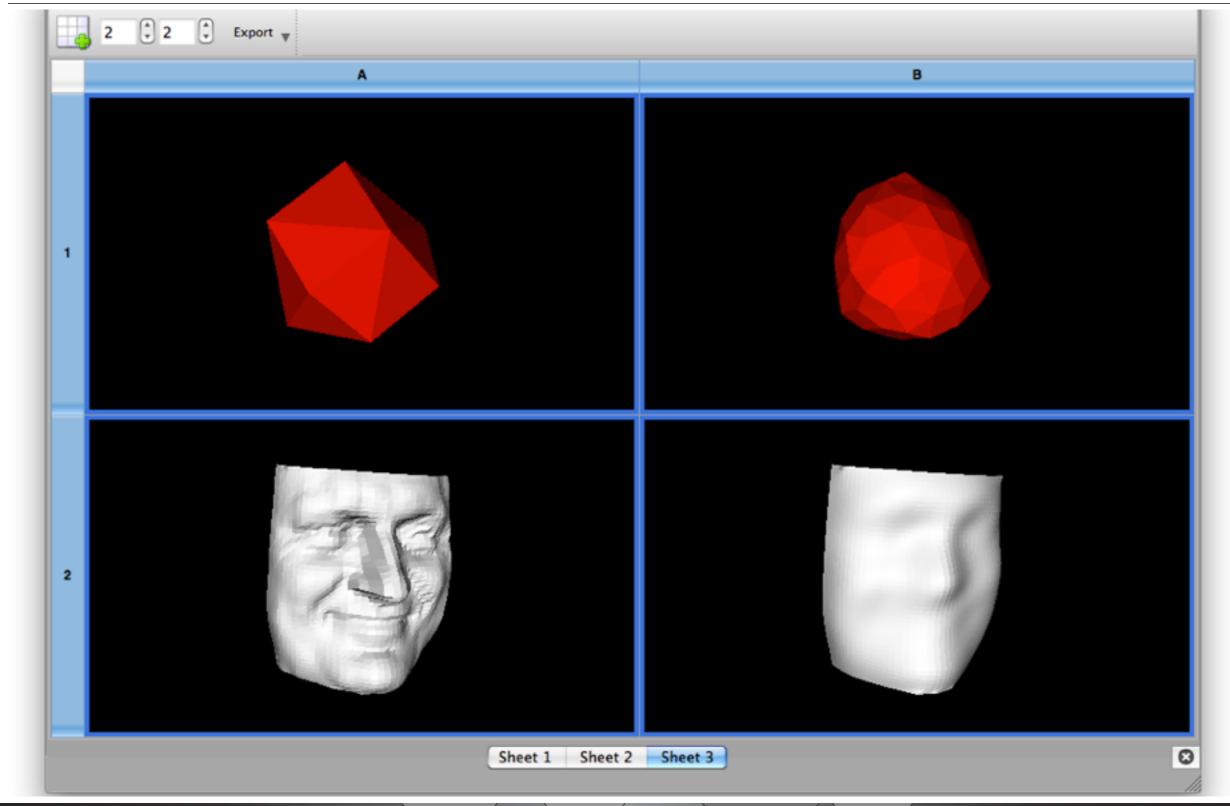


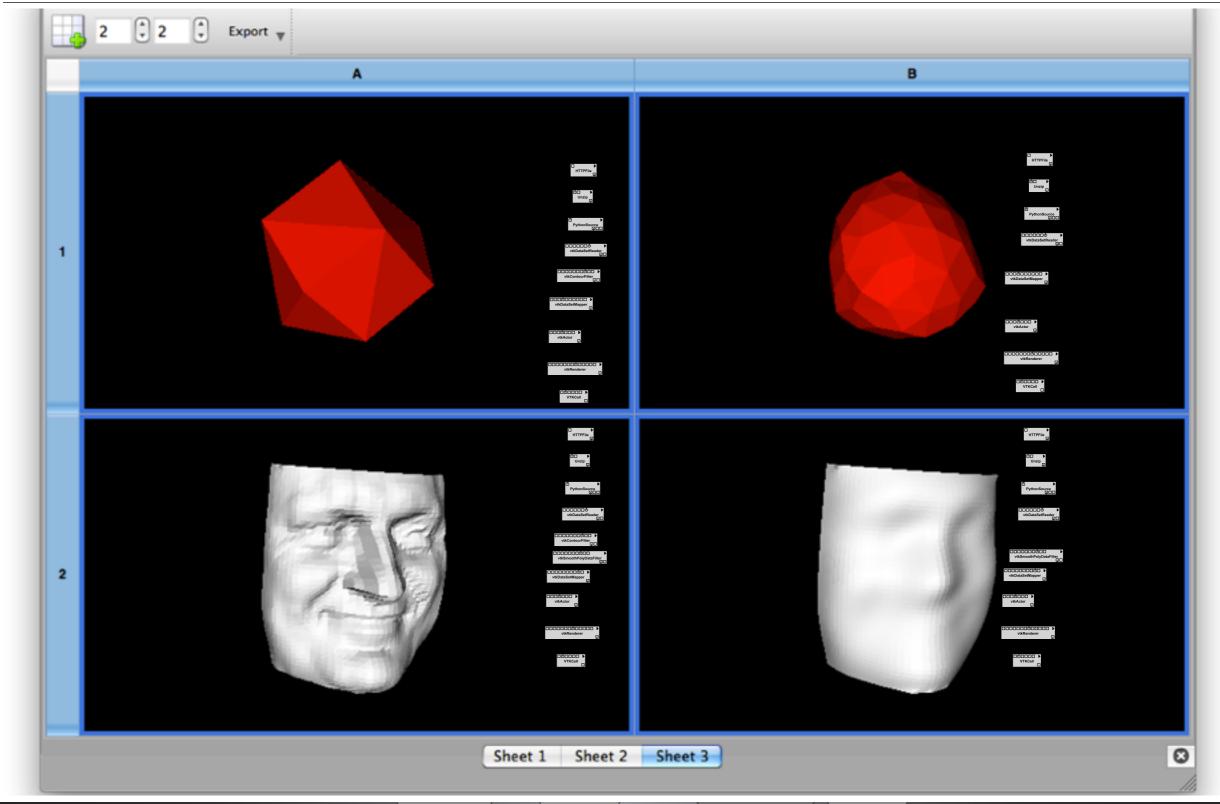
VisComplete Results

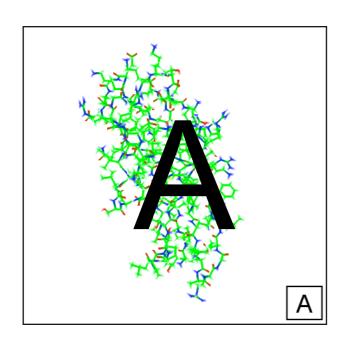




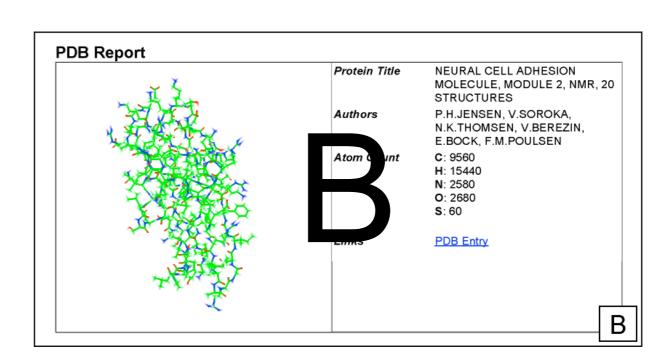




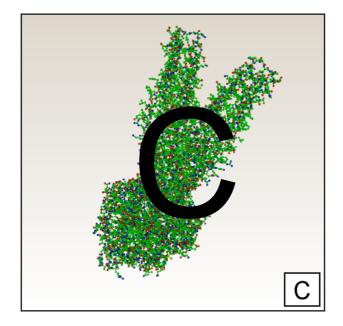




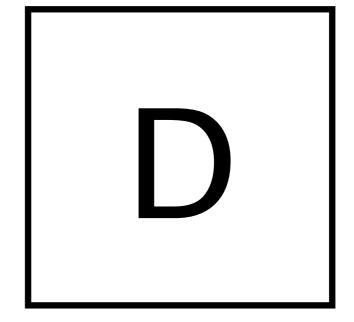
is to

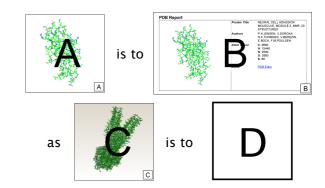


as

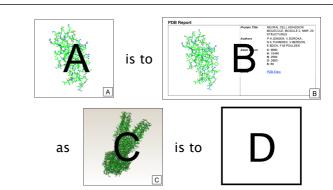


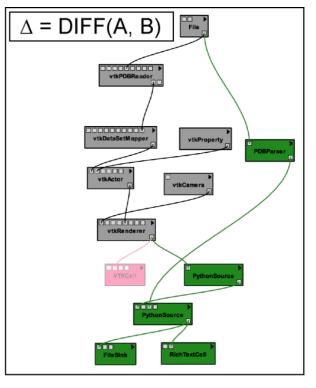
is to



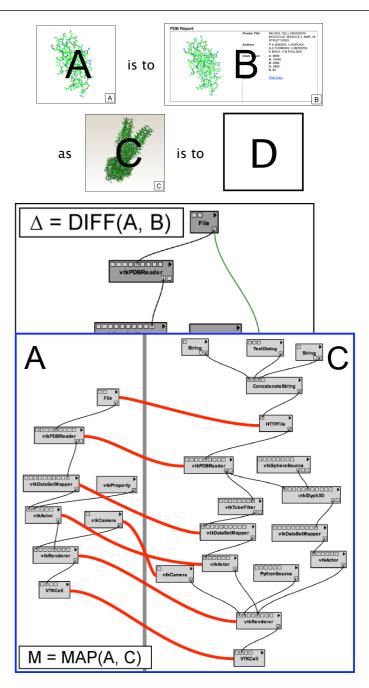


- Compute difference Δ(A,B) from provenance
 - D = Δ(A,B) C is often not a valid workflow

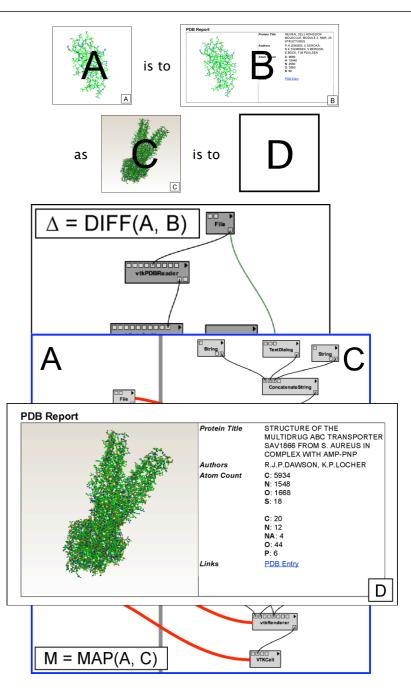




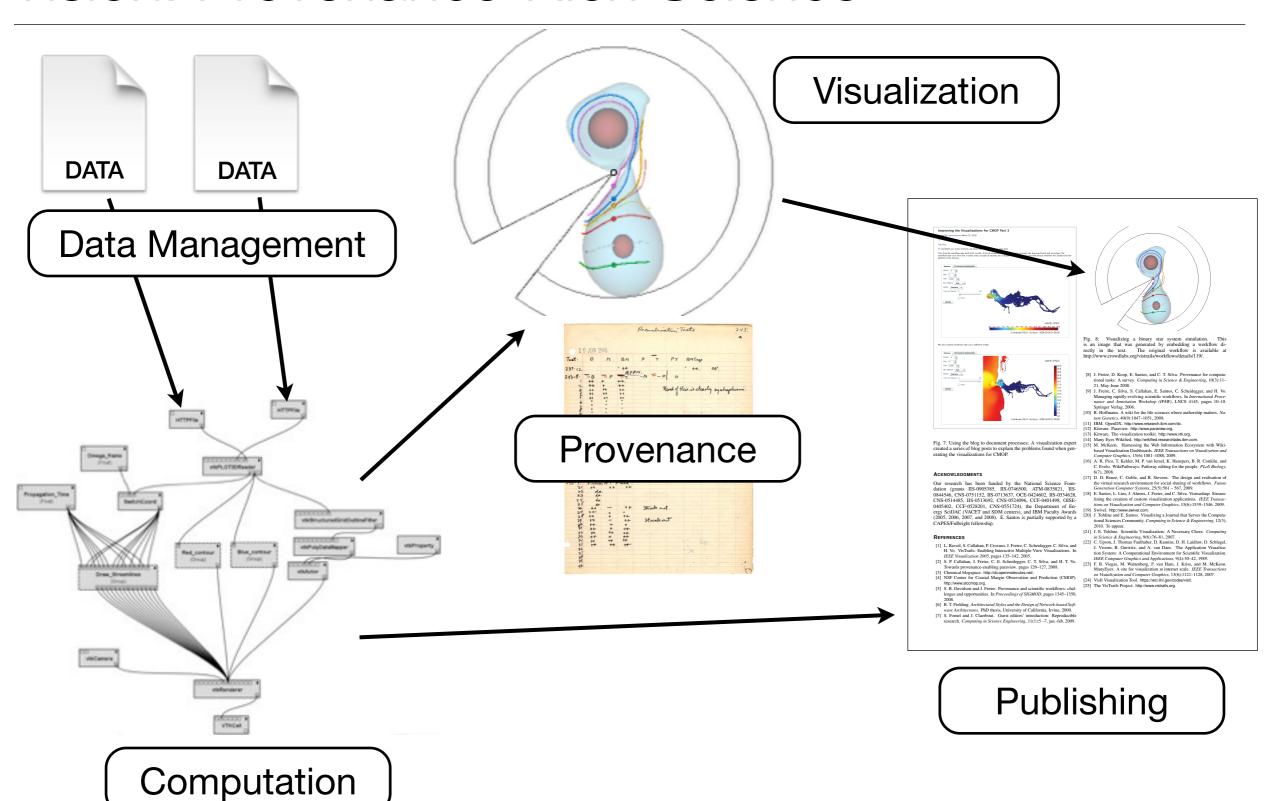
- Compute difference Δ(A,B) from provenance
 - D = Δ(A,B) C is often not a valid workflow
- Find map between A & C: map(A,C)



- Compute difference Δ(A,B) from provenance
 - D = Δ(A,B) C is often not a valid workflow
- Find map between A & C: map(A,C)
- Compute mapped difference
 ΔAC(A,B) = map(A,C) Δ(A,B)
 - D = \triangle AC(A,B) \circ C

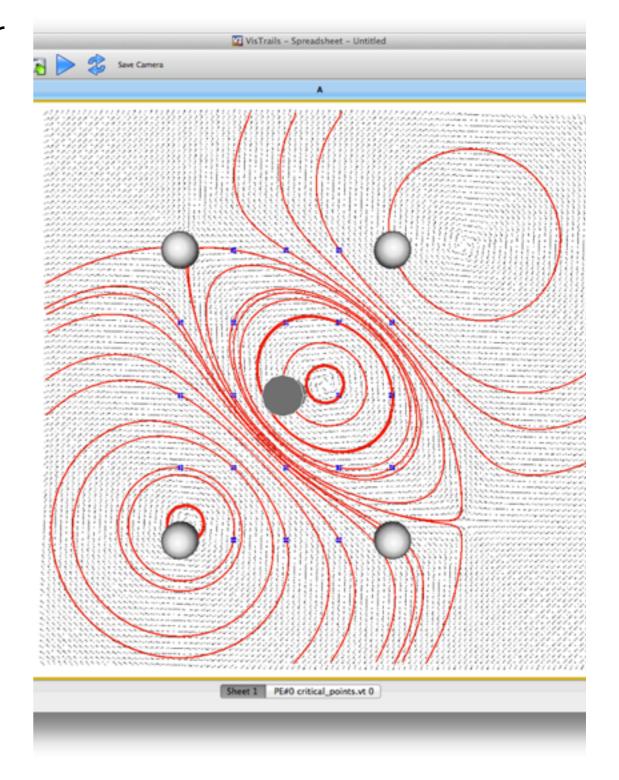


Vision: Provenance-Rich Science



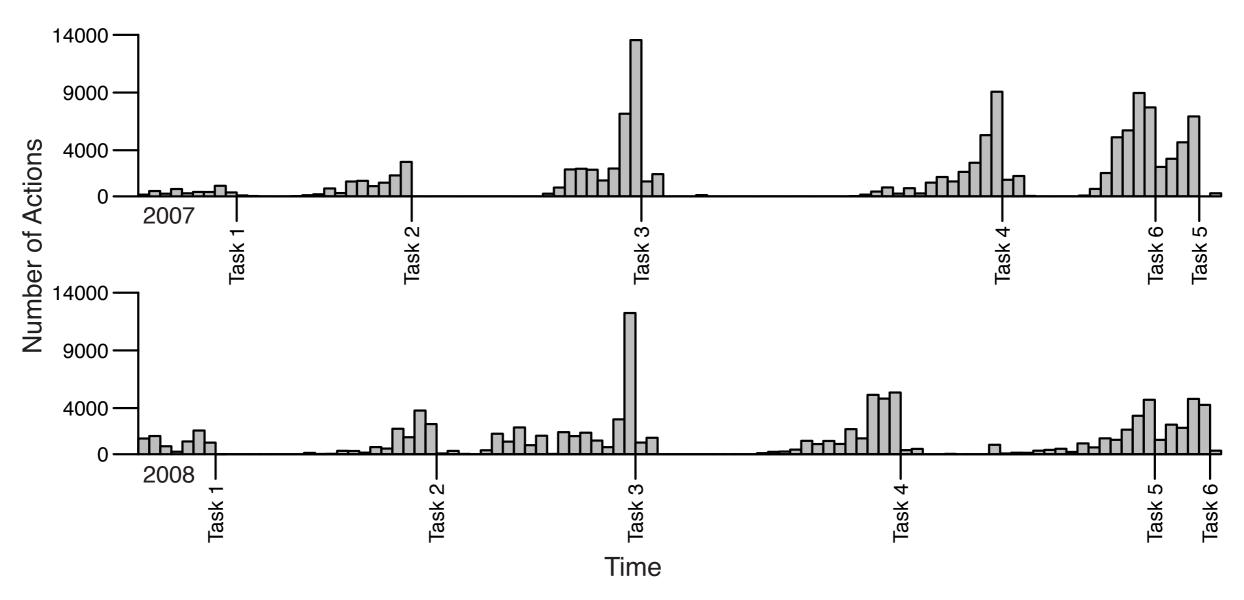
Provenance in Teaching

- "Using VisTrails and Provenance for Teaching Scientific Visualization" [Silva et al., 2010]
- Same features that scientists use for exploratory tasks can also benefit students
 - Exploration: see all pipelines not just a "final" one
 - Comparison: see different pipelines and what changes exist
 - Assessment: see how a solution was developed



Provenance Analysis of Projects

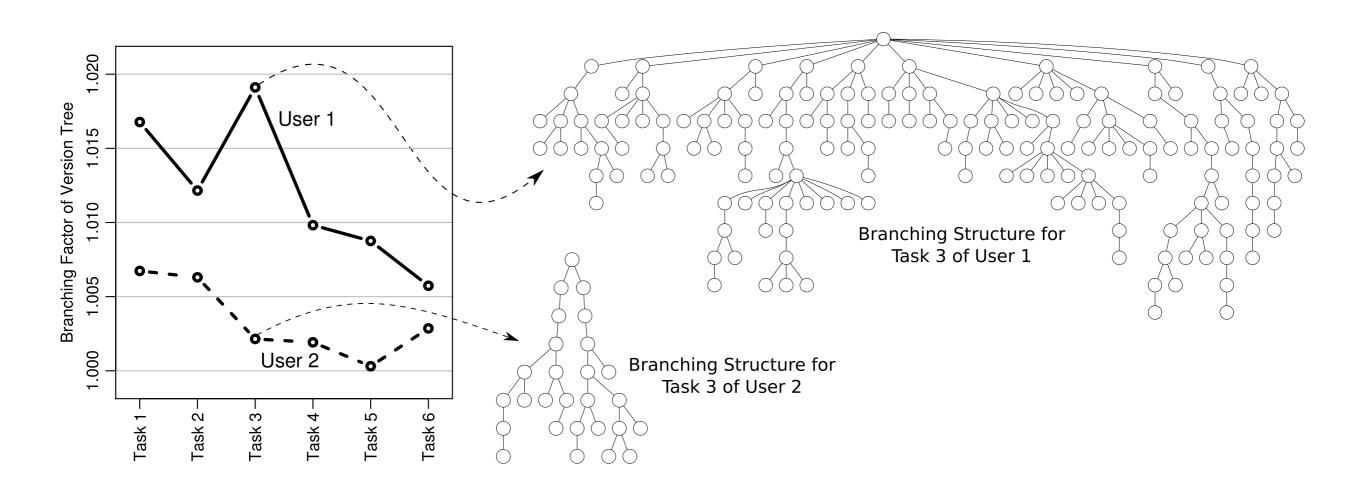
Activity Histograms by Date



[Lins et al., 2008]

Provenance Analysis of Projects

Comparing Paths to Solutions for Two Students



[Lins et al., 2008]

Conclusion: Uses of Provenance



Trust



Reuse



Reproducibility



Exploration

Conclusion: Take-Home Points

- Provenance is important
- Consider what needs to be stored, what would be nice to store, and what doesn't need to be stored
- Abstraction helps
- PROV model organizes and connects a variety of provenance
- Provenance isn't just for keeping a paper trail

Conclusion: References

- Bose and Frew: "Lineage Retrieval for Scientific Data Processing: A Survey"
- Simmhan et al.: "A Survey of Data Provenance in E-Science"
- Tan, "Provenance in Databases: Past, Current, and Future"
- Freire et al.: "Provenance for Computational Tasks: A Survey"
- PROV Model Primer: http://www.w3.org/TR/prov-primer/

Questions

